Nanoscale physics

Molecular dynamics simulations of the nanoscale droplet shape in the external force field

Mykola Isaiev[1,2], Sergii Burian[2], Leonid Bulavin[2], Michel Gradeck[1], Fabrice Lemoine[1], Konstantinos Termentzidis[1]

[1] *Laboratoire LEMTA, Faculté des Sciences et Technologies, CNRS UMR 7563, Université de Lorraine, BP 70239, 54506 Vandoeuvre les Nancy Cedex, France*
E-mail: mykola.isaiev@univ-lorraine.fr

[2] *Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Str., Kiev, 01601, Ukraine.*

Molecular dynamics is an efficient tool for the study and prediction of different properties at the nanoscale. In particular, it is successfully applied for the study of thermal conductance, elastic properties, viscosity etc. Especially, it is very useful for the investigation of the complex heterogeneous systems. However, it should be noted that the molecular dynamics simulations of the system with a huge numbers of atoms dramatically increase the computation time. Therefore, the simulations of the macrosized systems with molecular dynamics are problematic.

One should use physical laws that are invariant or predictable at the different scales to overcome this issue. As an example, the simulations of the wetting properties of liquid droplet on the solid substrate can be noted. Such, in [1] the statement that the wetting angle is the same for nanoscopic and for macroscopic cylindrical droplets was used. This allows us to evaluate the parameters of interaction between atoms of liquid droplet and solid surface.

In our report we will discuss the molecular dynamic simulations of the liquid droplet shape on the solid surface in an external force field. We correlate our results with the macroscopic model of the hydrostatic similarity. The region of the external field magnitudes for which the results of simulations are in good agreement with results obtained with the analytical model will be evaluated. Moreover, the mismatch between these results for the strong external field was explained in the terms of the adsorptions.

1. *Isaiev M., Burian S., Bulavin L., Gradeck M., Lemoine F., Termentzidis K.* Efficient tuning of potential parameters for liquid–solid interactions // Molecular Simulation. – 2015 (in print)