MODELING OF THE WETTABILITY OF NANOTEXTURED SURFACES BY THE METHOD OF MOLECULAR DYNAMICS

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Currently, micro- and nanodevices are actively developing, and the scope of their applications is aslo expanding. In this regard, the study of the influence of nanotexture geometry on near-surface processes is of great interest. One of this processes is wettability. When studying the wettability mechanism, difficulties arise, as well as measuring the contact angle at the micro- and nanoscale. To solve the above problems, it is proposed to use the method of molecular dynamics.

The aim of the work is to study the mechanism if wettability by the method of molecular dynamics to establish the influence of the material and geometry of surfaces on their wettability.

LAMMPS was used as a molecular dynamics package. The studied models included: a drop of water, TIP4P was used as a water molecule, a substrate consisting of copper, graphite or a composite using copper and graphene. The geometry of the substrate was determined either by a smooth surface or by a textured one constructed according to equation 1. The following values used as α and β parameters, respectively: 2, 4, 6 and 20, 40, 60.

$$z(x) = \alpha \sin(2\pi x / \beta). \quad (1)$$

The contact angle obtained an a copper substrate is ~10°, on graphite - 85°. When applying one layer if graphene to a copper substrate, the contact angle increases to 30°, with two layer – to 60° with three – to 85°. During the calculations, it was revealed that an increase in the β parameter can lead to both an increase in the contact angle and a decrease in it. When the α parameter was increased, the contact angle increased. There are also noticeable differences in the dynamic properties if the droplet. In a copper substrate, the droplet retains the horizontal position of the center of mass and spreads along the roughness. In turn, on graphite, the drop mainly retains its shape, and the center of mass moves along the surface of the substrate.

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