Thematic area of your work (one of the thematic areas of International research and practice conference "Nanotechnology and nanomaterials")

Temperature dependence of wetting angle of sessile droplet on the solid substrate by Molecular Dynamics Simulations

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Molecular Dynamics (MD) is a useful tool to investigate phenomena that occurred at the nanoscales and to predict several physical properties of different materials. However, the application of this method at the macroscale is limited mainly due to the computational cost. As an example, the evaluation of the wetting angle of sessile droplet could be mentioned[1–3]. Since the wetting properties at the nanoscale and macroscale significantly different, such evaluation is based on the serial changing of the droplet size and making of limit transaction for macrosize one. This method allows excluding the influence of line tension that change the wetting angle at the nanoscale. Recently, simulations with Monte Carlo method showed[4] that for the case of "infinity long droplet" there is the possibility to exclude directly the line tension influence and obtain the macrosize wetting angle.

In the current work, the study of the wetting properties of a liquid on a solid substrate with MD will be discussed. The simulations of the sessile water droplet on the silicon substrate will be given. The dependence of the wetting angle on the temperature for both the cases of spherical and cylindrical droplets will be compared. In addition, these dependences will be correlated with experimental data. Based on the analytical model the temperature dependences of the line and surface tensions of the liquid will be evaluated.

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2 *Barisik, M., Beskok, A.*: Wetting characterisation of silicon (1,0,0) surface // Mol. Simul.,-2013,-**39**, (January 2015), P. 700–709.

3 *Werder, T., Walther, J.H., Jaffe, R.L.*, *et al.*: On the Water - Carbon Interaction for Use in Molecular Dynamics Simulations of Graphite and Carbon Nanotubes // J. Phys. Chem. B,-2003,-**107**,-P. 1345–1352.

4 *Peng, H., Birkett, G.R., Nguyen, A. V.*: The impact of line tension on the contact angle of nanodroplets // Taylor & Francis,-2013,-40,-P. 934–941