Computer modeling the self-assembly of colloidal particles into evaporating sessile drop of water-glycerol solution

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The evaporating sessile drop of binary solution is an interesting object of theoretical and experimental investigations due to its important fundamental and practice applications. Recently, the concentration Marangoni driven migration of particles in such a system was experimentally investigated [1] There was experimentally shown that the polystyrene nanoparticles were moved by toroidal vortex flow acted inside a drop, and the direction of this flow depends on solvent components types (ethanol/water, isopropanol/water, metoxypropanol/water), ratio of mixture, particle size and environmental conditions. In such a system, the thermocapillary Marangoni number is much smaller than concentration Marangoni number $Ma_C = \frac{CR}{D\eta}\left|\frac{\partial\sigma}{\partial C}\right|$ (C is concentration of mixture component, R is drop radius, D is diffusion coefficient, η is viscosity, σ is surface tension), so that the concentration gradient is a main origin of Marangoni instability.

In our case, colloidal nanoparticles self-assembly into evaporating sessile drop of binary solvent mixture water-glycerol ($C_3H_5(OH)_3$) deposited on a flat substrate is considered. The components of such a solvent have highly contrasting properties. Under normal conditions, pure liquid water has approximately a 10 000 times higher evaporation rate and viscosity a 1000 times less than pure glycerol has.

Recently, we developed the evaporation model of sessile drop of binary solvent mixture (with infinitely soluble in each other components) based on Hu and Larson solution for single solvent sessile drop and Raoult law for saturated vapor density of components of binary mixture in wide range of unidimensional molar binary concentration of the components. (The Raoult law declares that saturated vapor density of first component has a linear reducing dependence on the percent of second component presence in binary solution if this addition of second one is small enough) [2].

In this report we suggest a new physical model of dissipative particle dynamics (DPD) in drop of binary solvent mixture as a further development of recently elaborated DPD model of self-assembly into evaporating droplet of pure solvent [3] with account of phenomenological results obtained in our experiments. The output data include the trajectories of particles during drop evaporation process. The computer modeling results are compared with the previously mentioned experiments.

[1] E. L. Talbot, A. Berson, L. Yang and C. D. Bain, Internal Flows and Particle Transport Inside Picoliter Droplets of Binary Solvent Mixtures. NIP 29 and Digital Fabrication. Book of Abstracts, 307 – 312 (2013)

[2] P. Lebedev-Stepanov, A. Kobelev, S. Efimov. Evaporation dynamics and Marangoni number estimation for sessile picoliter liquid drop of binary mixture solution/ MATEC Web of Conferences – 2016. – V 84, 22. - P. 1-4.

[3] P.V. Lebedev-Stepanov and K.O. Vlasov, Simulation of self-assembly in an evaporating droplet of colloidal solution by dissipative particle dynamics, Colloids and Surfaces A : Physicochem. Eng. Aspects. 432, 132-138 (2013).