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Simulation of self-assembly in an evaporating inkjet-sized droplet of colloidal solution by dissipative particle dynamics

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A method of Brownian dissipative dynamics of charged colloidal nanoparticles in microdroplet of solution deposited on plane substrate is proposed for investigation of self-assembly and self-ordering of colloids during solute evaporation. Method is based on the numerical solution of multi-scale Langevin equation for each particle, the hydrodynamic microflows approach, and droplet evaporation model. It takes into account the DLVO-forces between the particles, their interaction with the substrate (adhesion, friction, and roughness); Stokes', Brownian, and capillary forces (wetting and depinning, outflow angles, and surface tension). The nature of coffee ring effect was studied. It is shown that the hexagonal domain ordering of particles ensemble in pattern can be formed onto plane substrate as a result of interparticle repulsion and the capillary compression during evaporation of solvent. Numerical results are in good agreement with inkjet technology experiments. Modeling demonstrated that by the varying roughness, surface adhesion, wettability and other parameters, it is able to control the degree of ordering of the solid phase, formed as a result of particles self-assembly in an evaporating microdroplet.

Biography

Peter V. Lebedev-Stepanov, Ph.D., Physics and Mathematics now is an associate Professor of Physics at National Research Nuclear University 'MEPhI' (since 2009), head of the Research Laboratory of self-organization of nanoparticles and photonics of nanostructured patterns at Photochemistry Center of Russian Academy of Sciences (since 2007). His researches focus on the statistical physics and physical chemistry of open systems, self-organizations, computer simulations of properties of charged nanoparticles and their ensembles, and interaction of colloids in solution. He has more than 120 scientific publications.

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