Nanocomposites and nanomaterials

Study of the dynamics of formation of spatial nanostructures

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Nanostructure formation processes in disperse systems play an important role in the creation of new materials and systems with unique thermalphysic and physicochemical properties that determine their functional properties [1].

A two-level modelling method, based on Molecular Dynamics (MD) method and Dissipative Particle Dynamics (DPD) method is used for theoretical studies of the dynamics of structure formation in superdispersed systems [2].

The using of the MD method allows taking into account intermolecular forces in the dispersion medium (fluid). A DPD method is used to calculate the interaction of nano-dispersed particles of the dispersion medium and the particles together, considering the attractive forces that are responsible for structure formation processes.

The applied method of calculation allows to predict the shape of the spatial structure (spherical, "wormlike", globular, etc.).

The experimental and calculated structures in the dispersion «nanoscale silicon dioxide - water» were compared and showed that there were distinctively globular structures of nanoparticles in the two cases. This correlation allows to conclude the efficiency of the proposed model for the analysis of structure formation processes.

1. *Uriev N.B.* Physico-chemical dynamics of structured nanodisperse systems / / Physical Chemistry of Surfaces and Material Protection. -2010.-**46,** NN 1,3**.**-P. 3-23, 227-241.
2. *Dzwinel W., Yuen L.A.* A two–level, discrete particle approach for large – scale simulation of colloidal aggregates // Int. Journal of Modern Physics.-2000.-**11**, N 5.-P. 1037–1061.