A self-assembly of nanoparticles

Yushchenko O.V., *Associate Prof.r*; Badalyan A.Yu., *Assistant*;
Bratash S.O., *Stud.*
Sumy State University, Sumy

Nanotechnology achievements are often connected to material science because the design of a wide range of advanced nanostructured materials will reduce the size of the components of many devices. But nanoscience today is more interested in the formation of nanoassemblies and further coupling of them into the nanostructured materials.

There are two main methods of nanoassemblies fabrication: top-down and bottom-up. While the first method is based on different types of lithography, the second method is characterized by the self-organization process – self-assembly of atoms or molecules. Self-assembly involves a large number of nanoparticles, occurs parallel, and forms hierarchically structured materials. So for design of materials with desired properties the self-assembly becomes the most promising method.

Wepropose amodel of the self-assembly of active nanoparticles on the basis of the canonical Hamiltonian approach. Considering the coordinate, momentum and internal energy of the particle, we arrive to the system of three differential equations. For the adiabatic approximation it is reduced to a system of two differential equations, which was investigated by the phase-plane method.

Within our approach all equilibrium states are realized at zero momentum. But depending on the system parameters and the internal energy given by the external conditions, these states may be stable (then particles with the corresponding initial values of coordinate and momentum move to this point) or unstable (the nearest particles change their coordinate and momentum so that move away from the given point). Besides the transformation of internal energy has a big impact. If the internal energy is transformed only into kineticenergy, then there are two possible stable states (two coordinates, where the self-assembly occurs. If the internal energy is transformed not only into kinetic energy, but also into potential energy, much more stable states are realized. But the sensitivity to the initial conditions increases.Analyzing the obtained results, we can talk not only about the possibility of nanoparticles' self-assembly, but also about the coordinates and the velocity of the process realization.