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Computer Simulation of Self-assembly of Structure from an Ensemble of Nanoparticles

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Abstract. Self-assembly is one of the methods utilized to create intricate geometry-based structures at the nanoscale. Earlier research in this field has shown that the formation of multiparticle structures using this technique is primarily achievable through gradual assembly, where a new particle is connected with a previously formed cluster. But step-by-step construction requires additional expenses and may result in defects within the already formed structures. If step-by-step assembly is not appropriate, a structure can be formed from a ensemble of particles without additional influence, but it is uncertain whether the probability of structure formation and the process selectivity are high. The paper presents a mathematical model that demonstrates how to derive a structure from an ensemble of particles, describes its implementation through software, and proposes the result of computational experiments.

Keywords: mathematical model, nanostructure self-assembly, computational experiment, Langevin dynamics.

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Introduction

Scientific and technological interest is heightened in terms of the study of nanometric structures and their application in the creation of devices [1]. This is especially important in electronics, where smaller components allow for smaller devices with faster signal transmission. At the same time, many-particle systems play an important role in the description of many processes, the elements of which interact with each other through the environment, represented by both physical and chemical characteristics and a superposition of forces acting on the ensemble. Here there is an important feature for multiparticle systems: when faced with forces that affect the ensemble directly or indirectly through the environment, some particles can aggregate into structures. The term self-organization or self-assembly is used to describe such a process [2].

Self-assembly processes are the subject of theoretical and experimental studies in many application. The area of practice application is related to the binary solvents, mixing different kinds of particles, creating multilayer systems, achieving multistage self-assembly, and controlling the self-assembly of external fields, such as, for example, inertial forces [3–5]. The use of self-assembly is especially interesting for describing the aggregation of ultrasmall nanoparticles, like nanodiamonds [6, 7], quantum dots and supramolecules [8], and metal particles [9]. There is much

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less work on theoretical modeling of such systems. Molecular Brownian dynamics, Monte Carlo methods, dissipative particle dynamics, and self-consistent field theory are commonly utilized as tools for mathematical and numerical modeling to explore self-organizing structures.

From the point of view of mathematical and computer modeling of self-assembly processes, the most important is the construction of physically meaningful and computationally simple models. The choice of model is determined by the approximations necessary to simplify the initially complex phenomenon. The existing experience of the authors in the application of Brownian particle dynamics for modeling self-assembly processes in the volume of a solution indicates the possibility of reproducing and predicting real processes and phenomena in both simple and more complex systems. Thus, earlier in [10,11], an universal method was proposed for the formation of nanostructures under the action of an external quasi-resonant field due to the self-organization of nanoparticles. The first experiments [12,13] showed the fundamental possibility of pair formation from colloidal quantum dots. Numerical calculations [14] showed the possibility of creating more complex structures using staged self-assembly. This work is devoted to a mathematical and computer model of self-organization of aggregates from an ensemble of particles for estimating the parameters of the medium and field at which such an assembly becomes possible, as well as to a numerical analysis of the simulated process.

The article is organized as follows. Section 2 is devoted to the mathematical formulation of the problem and its implementation. Section 3 presents the results of computational experiments. Section 4 proposes conclusions and discussion of the results.

1. Mathematical formulation

Assume that under laser radiation field an ensemble of N nanoparticles having mass m_j of radius R_j and resonant frequency $\omega 0_j$, $j = 1, \ldots, N$ is considered. For every $j-$th dipole particle at any moment in time, we define:

$\bar{r}_j = \left(r_j^x, r_j^y, r_j^z\right)$ – radius-vector of the particle's center of mass;

$\bar{v}_j = \left(v_j^x, v_j^y, v_j^z\right)$ – vector of translational velocity of the particle's center of mass;

$\bar{\omega}_j = \left(\omega_j^x, \omega_j^y, \omega_j^z\right)$ – particle rotational velocity vector;

$\bar{d}_j = \left(d_j^x, d_j^y, d_j^z\right)$ – dipole moment vector.

The problem is to estimate the probability of assembling structures from an ensemble of particles for fixed parameters of the medium and field, in a time not exceeding the duration of one laser pulse ($T \leqslant 10$). The difference from our previous works lies in the solution of a multiparticle problem, when we are not limited to step-by-step assembly or a small number of particles (for example, see [14]). Here we are primarily interested in the possibility of assembling structures consisting of more than two particles and the selectivity of the process.

1.1. Langevin dynamics to describe the motion of an ensemble of particles

In this section we briefly describe the model used to describe many-particle interactions. It is based on a description of interaction through Langevin dynamics, a physical concept developed for statistical modeling of molecular systems. It represents stochastic dynamics in which particles move under the influence of a force directed towards the most probable regions of state space, determined by the parameters of the environment. To avoid repeating complete model conclusions regarding our previous works for pairs and triplets of particles [14,15], only the main equations and comments regarding the many-particle problem will be given here.

a) translation motion

Let us separately describe the translational and rotational motion of an ensemble of particles. Given that the ensemble size is much smaller than the wavelength of the incident radiation, we can assume that the external electric field $\vec{E}$ is uniform

$$\vec{E} = 1/2\ \vec{E}_0 \exp(i\omega^r t) + c.c.$$

and not to take into account delays. Here ω^r is the frequency of laser radiation. One of the widely used methods for describing the translational motion of an ensemble of particles is Langevin dynamics [11], expressed in the form of system

$$\begin{cases} d\bar{r}_j/dt = \bar{v}_j, \\ m_j d\bar{v}_j/dt = \bar{F}_j, \end{cases} \tag{1}$$

where $\bar{F}_j$ is the superposition of forces acting on the j-th particle, including friction forces and stochastic forces that take into account the temperature parameters of the medium. As the $\bar{F}_j$ we will consider the sum of the following components

$$\bar{F}_j = \vec{F}_j^v + \vec{F}_j^e + \vec{F}_j^d - \vec{F}_j^f + \vec{F}_j^c, \tag{2}$$

where $\vec{F}_j^d = -\nabla(W_j^d)$ is the electrodynamic force; $\vec{F}_j^v = -\nabla(W_j^v)$ is van der Waals force; $\vec{F}_j^e = -\nabla(W_j^e)$ is electrostatic repulsion force; $\vec{F}_j^f$ is viscous friction force; $\vec{F}_j^c$ is stochastic hydrodynamic force. Here $W_j^d, W_j^v,\ W_j^e$ are the energies of dipole-dipole, van der Waals and Coulomb interactions of an ensemble of particles at the position point of that particle, determined by (3)–(5) respectively.

$$W_j^d = \frac{1}{4\pi\varepsilon_0} \sum_{k\neq j} \frac{(\vec{d}_j, \vec{d}_k)|\vec{r}_{jk}|^2 - 3(\vec{d}_j, \vec{r}_{jk})(\vec{d}_k, \vec{r}_{jk})}{|\vec{r}_{jk}|^5}; \tag{3}$$

$$W_j^v = -\frac{A_H}{6} \sum_{k\neq j} \left(\frac{2{R_j}^2}{h_{jk}^2 + 4R_j h_{jk}} + \frac{2{R_j}^2}{h_{jk}^2 + 4R_j h_{jk} + 2{R_j}^2} + \ln \frac{h_{jk}^2 + 4R_j h_{jk}}{h_{jk}^2 + 4R_j h_{jk} + 2{R_j}^2} \right); \tag{4}$$

$$W_j^e = 2\pi\varepsilon_r\varepsilon_0 R_j {\phi_0}^2 \sum_{k\neq j} \ln\left[1 + \exp(-h_{jk}k_0)\right]. \tag{5}$$

Here A_H is the Hamaker constant; h_{jk} is interparticle gap; ϕ_0 is potential at the Helmholtz boundary; ε_r is dielectric constant of the medium; k_0 is screening constant.

For spherical particles the Stokes formula allows calculate the force of viscous friction $\vec{F}_f$

$$\vec{F}_j^f = 6\pi\eta R_j \vec{v}_j, \tag{6}$$

where η is the dynamic viscosity of the medium. The interaction of particles with a medium with fluctuating density usually leads to a random change in their trajectory. To take Brownian motion into account, consider a random force $\vec{F}_j^c$ described by a Gaussian distribution. Suppose a particle or particle's cluster experiences a random force over Δt. Before each integration step, the values of the projections of the random force $\vec{F}_j^c$ on the coordinate axes are selected from a Gaussian distribution with zero mean and standard deviation $\sigma^2 = 12\pi\eta RkT/\Delta t$.

b) rotational movement

The rotational motion of an ensemble of particles, arising as a result of the interaction of particles with induced dipole moments $\vec{d}_j$ in a uniform constant laser field in a viscous environment is determined by the action of the torque $\vec{N}_j$:

$$\vec{N}_j = \left[\vec{d}_j \times \vec{E}\right] + \vec{M}_j^{rot}, \tag{7}$$

where $[\vec{a} \times \vec{b}]$ is the vector product and $\vec{M}_j^{rot}$ is the torque caused by the forces of hydrodynamic resistance to the rotation of the structure

$$\vec{M}_j^{rot} = \left[\vec{F}_j^{tr} \times \vec{r}_j\right],$$

where $\vec{F}_j^{tr}$ is the superposition of forces acting on the particle with the exception of the force of electrodynamics interaction. One of the techniques to describe the rotation of a structure mathematically involves identifying it with rotation by a moving (local) coordinate system, which is fixed to the structure. For the connection between the moving and inertial coordinate systems, Euler angles are considered [15]. Using the equation of moments [16], we determine the rotation of the structure in the local coordinate system according to the presence or absence of momentum.

$$\frac{\mathrm{d}\vec{L}_j}{\mathrm{d}t} + \left[\vec{w}_j^{loc} \times \vec{L}_j\right] = \vec{N}_j^{loc}. \tag{8}$$

Here $\vec{L}_j$ is the angular momentum of the dipole structure, defined as $\vec{L}_j = J_j \vec{w}_j^{loc}$; $\vec{N}_j^{loc}$ is the rotational moment determined in the local coordinate system (CS). The position of the moving CS relative to the inertial one is determined by Euler's kinematic equations [16].

Remark 1. The initial distribution of dipole moments can be determined from a system of linear algebraic equations:

$$\vec{d}_j = \mathcal{X}_{0j}\left(\vec{E} + \sum_{k \neq j} \vec{E}_k\right),$$

where $\mathcal{X}_{0j}$ is the linear polarizability of j-th isolated particle, $\vec{E}_k$ is the field created by that particle of the ensemble at the location of k-th particle [15].

Remark 2. The "gluing" of particles into a pair or the formation of more complex multiparticle structures was considered to be the achievement of an interparticle gap between the gluing components of less than half the radius of the particle. After gluing, the center of mass of the formed structure is determined depending on the geometric arrangement of the particles forming it; mass as the sum of the masses of the parts forming the structure and dipole moment as a superposition of the forming dipole moments.

Remark 3. When modeling the translational motion of structures consisting of several nanoparticles, the same formulas (1)–(6) were used as for an ensemble of particles, except for the Stokes formula for calculating viscous friction forces for formed pairs of particles. Instead, we used the approximation of the pair by a cylinder of the appropriate radius and a generalization of the Stokes formula proposed in [15]. In turn, rotational motion for pairs of particles and more complex agglomerates, in contrast to isolated particles, requires the introduction and consideration of a local CS, rigidly related to the structure. Technical issues of modeling the rotation of a pair are discussed in [15].

1.2. Numerical solution and system scaling

For the numerical implementation of the system of differential equations, the Runge–Kutta method of the 4-th order was used. For the simulation, we considered an ensemble of CdTe particles in an aqueous solution. The parameters of particles, medium and field are described in Tab. 1. Note that the program for modeling the interaction of dipole particles is implemented in the C++ programming language, and the maximum accuracy of representing a real number during operation is ensured by the double type and is 15 significant digits. Therefore, it is necessary that the ratio of the maximum number to the minimum number does not exceed 10^{15}. Based on this restriction, we scaled the basic units of measurement of the International System of Units (SI):

$$\text{m} = 10^9\ m^*;\ \text{kg} = 10^{23}\ kg^*;\ \text{s} = 10^9\ s^*;\ \text{A} = 10^{13}\ A^*.$$

The values of the corresponding scaled quantities with descriptions and initial values are presented in Tab. 1.

Table 1. Description of constants and scaled quantities

Description	**Designation**	**Value**	**Scaled value**
Particle radius	R	$1.5{\cdot}10^{-9}\ m$	$1.5\ m^*$
Particle mass	m	$8.2485{\cdot}10^{-23}\ kg$	$8.2485\ kg^*$
Planck's constant	$\hbar$	$1.054{\cdot}10^{-34}\ J\cdot s$	$1.054\cdot 10^{-2}\ J^*\cdot s^*$
External field wavelength	λ	$690{\cdot}10^{-9}\ m$	$690\ m^*$
Resonance wavelength	λ_0	$525{\cdot}10^{-9}\ m$	$525\ m^*$
Uniform line width	G	$1.6{\cdot}10^{13}\ Hz$	$1.6\cdot 10^4\ Hz^*$
Dielectric constant in vacuum	ε_0	$8.82{\cdot}10^{-12}\ F/m$	$8.82\ F^*/m^*$
Relative dielectric constant of water	ε_r	81	81
Potential at the Helmholtz boundary	ϕ_0	$2.34{\cdot}10^{-3}\ V$	$2.34\cdot 10^{-2}\ V^*$
Viscosity	η	$0.8902{\cdot}10^{-3}\ Pa\cdot s$	$0.8902\cdot 10^2\ Pa^*\cdot s^*$
Screening constant	k_0	$0.1{\cdot}109\ m^{-1}$	$0.1\ m^{*-1}$
Boltzmann's constant	k_b	$1.38{\cdot}10^{-23}\ J/K$	$1.38\ J^*/K^*$
Hamaker constant	A_H	$50k_bT$	$50k_bT$
Transition dipol moment in a two-level system	$\lvert d_{12}\rvert^2$	$1.91\cdot 10^{-44}\ J\cdot m^3$	$19.1\ J^*\cdot m^{*3}$
Temperature	T	$300\ K$	$300\ K^*$
Speed of light	$_0$	$2.99{\cdot}10^8\ m/s$	$2.99\cdot 10^8\ m^*/s^*$
Field intensity	I	$10^{10}\ W/m^2$	$10^6\ W^*/m^{*2}$
Electric field strength	$\lvert\vec{E}\rvert$	$2.27{\cdot}10^6 V/m$	$2.27\cdot 10^{-2}\ V^*/m^*$

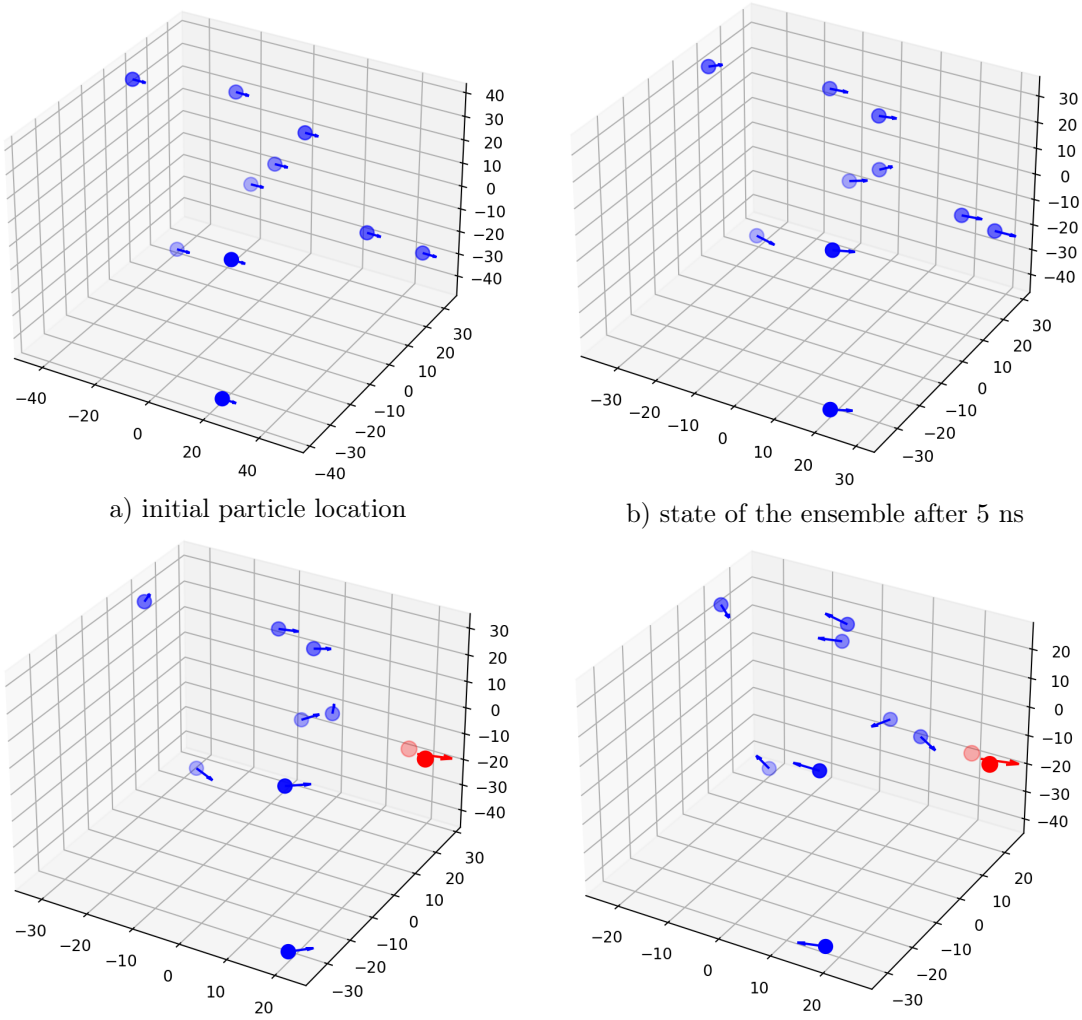
Assume also that in Cartesian coordinates the electric field strength vector $\vec{E} = (E^x, E^y, E^z)$ is determined by the radiation intensity and two angles α and β as follows:

$$\begin{cases} E^x = E\sin\alpha\sin\beta, \\ E^y = E\sin\alpha\cos\beta, \\ E^z = E\cos\alpha. \end{cases} \tag{9}$$

2. Results of numerical simulation

Fig. 1 shows an example of modeling the interaction of an ensemble of dipole particles for 10 ns from 10 particles. The initial location of the particles was set randomly within the cube with a 100 nm edge. As a result of the simulation, a pair is formed at 7 ns. No other structures were formed.

Fig. 2 shows the probability of assembly of at least one structure depending on the direction of laser radiation for different numbers of particles in 10 ns. Note that structures other than pairs were not formed for any combination of angles and initial numbers of particles. Fig. 3 shows the dependence of the average assembly time of the first pair of particles on their initial number. Fig. 4 shows a visualization of the change in the probability of structure assembly with an increase in the initial number of particles in the system at certain angles of incidence of laser radiation.



a) initial particle location

b) state of the ensemble after 5 ns

c) assembly in pair at 7 ns

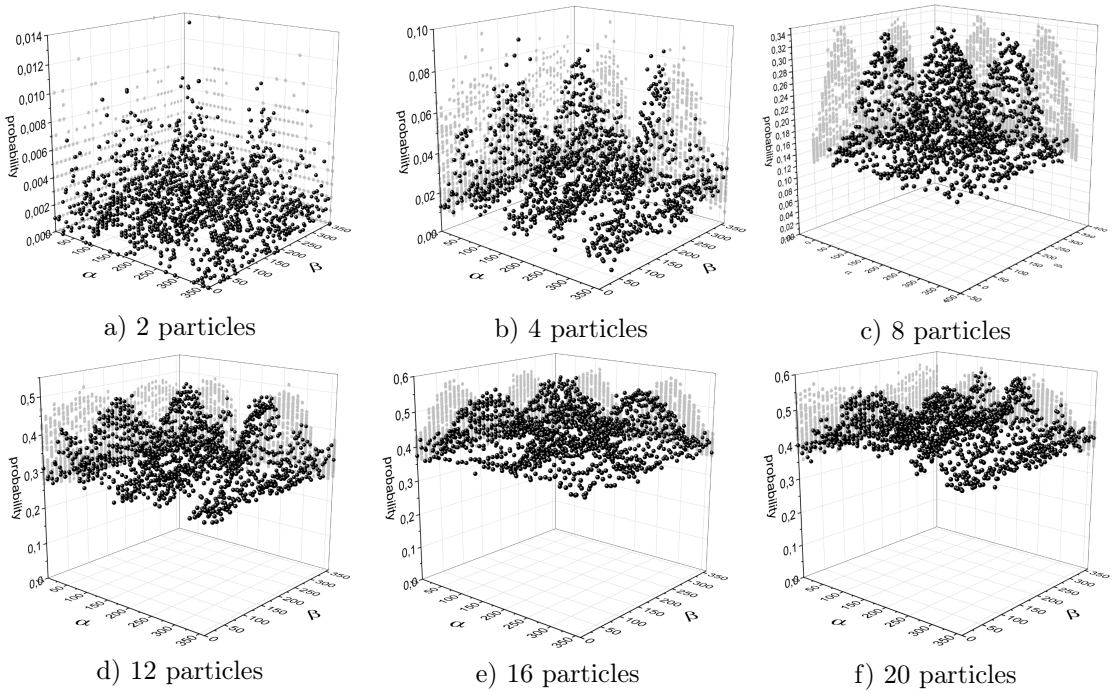
d) state of the ensemble after 10 ns

Fig. 1. An example of modeling the interaction of an ensemble of 10 dipole particles

3. Conclusions and discussion

The article is devoted to a numerical assessment of the possibility of self-assembly of agglomerates from an ensemble of nanoparticles under certain environmental and field parameters. Previously obtained results, described, for example, in [12–14], show that with certain conditions of the environment, self-organization of particles of a given geometry becomes possible. It was shown that the probability of such an assembly depends significantly on the initial distance between particles. The described difficulty can be overcome by changing the concentration of particles, which, in the presence of random fluctuations, leads to the assembly of structures. However, it remained not obvious whether the process stay selective with respect to the field parameters, for which purpose the corresponding computational experiments were carried out. To implement the assessment, a mathematical model was built, described in Section 2.

Briefly describe the obtained results. Figures 2 and 4 show that, regardless of the initial number of particles, the maximum probability of assembly is achieved when the laser is positioned



a) 2 particles b) 4 particles c) 8 particles

d) 12 particles e) 16 particles f) 20 particles

Fig. 2. Probability of pair assembly depending on the direction of laser radiation for different numbers of particles in 10 ns

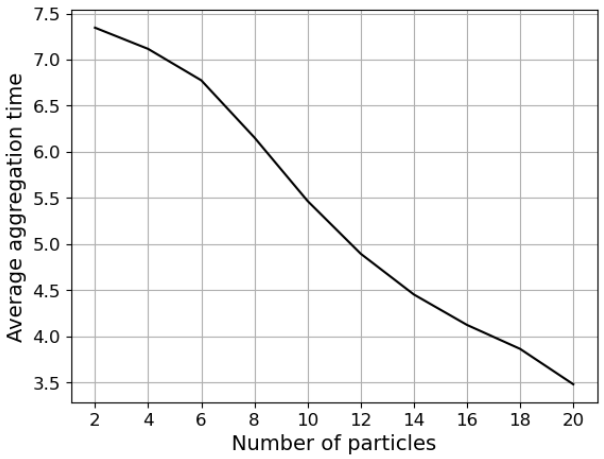
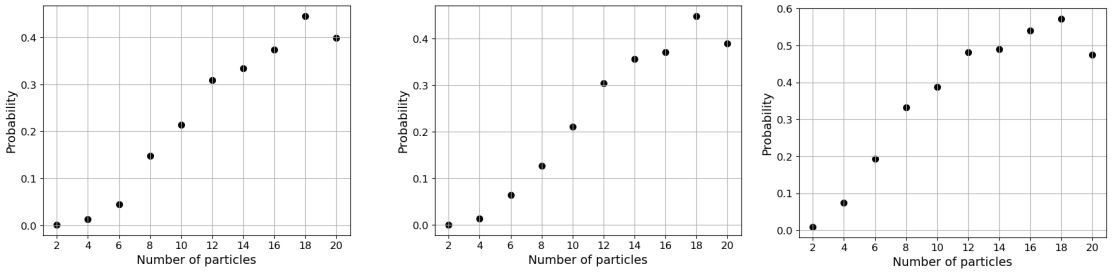


Fig. 3. Dependence of the average assembly time of the first pair of particles on their initial number

along the x axis, while with a different direction of the laser beam, assembly also occurs, but with a lower probability. Note that, due to the symmetry of the process, there should be no obvious advantage in the direction of laser radiation for assembly, that is, at high concentrations and random arrangement of particles, the process should be non-selective in the direction of laser radiation. This phenomenon most likely arises due to the peculiarities of the software modeling, since the initial location of particles along the y, z axes was chosen randomly throughout the entire



a) $\alpha = 0;\ \beta = 0$ b) $\alpha = 90;\ \beta = 0$ c) $\alpha = 90;\ \beta = 90$

Fig. 4. Probability of structure assembly for different numbers of dipole particles for certain field parameters

computational domain, and along the x axis — in a narrower part of the domain, depending on the number of particles so that nanoparticles occupied the computational space area uniformly. This was done so that when the area was randomly filled, it did not occur that some particles were generated already at the distance at which gluing was performed. Note that from Figures 2 and 4 it is clear that the difference between the maximum and minimum probability of aggregation narrows with increasing particle concentration.

We also note that at the chosen wavelength of the external field, corresponding to the assembly of pairs of particles [12], structures other than pairs are not assembled. In this case, with an increase in the number of particles in the ensemble, the growth rate of the assembly probability slows down, as can be seen from Fig. 4. This can be explained by the superiority of the electrostatic repulsion forces over the electrodynamics interaction forces at a small interparticle gap, as was shown in [13]. Note also that at $N = 20$, the average distance between particles along one axis is of the order of the particles' diameter, where the use of the dipole-dipole approximation becomes incorrect. Fig. 3 shows a similar behavior of the average assembly time of the first pair depending on the initial number of particles.

Thus, the results of computational modeling demonstrated the possibility of self-assembly of pairs from an ensemble of free isolated dipole particles with a high probability exceeding 50% at high concentrations in the volume. At the same time, the problem of the possibility of assembling more complex structures from an ensemble of particles and pairs, as well as taking into account relaxation processes when turning off laser radiation, remains a question for future research.

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Компьютерное моделирование самосборки структур из ансамбля наночастиц

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Аннотация. Самосборка — один из методов, используемых для создания сложных геометрических структур на наноуровне. Более ранние исследования в этой области показали, что формирование многочастичных структур с использованием этого метода в первую очередь достижимо путем поэтапной сборки, когда новая частица присоединяется к ранее образованному кластеру. Но поэтапное формирование требует дополнительных затрат и может привести к дефектам уже полученных конструкций. Если поэтапная сборка невозможна, то структура может быть сформирована из ансамбля частиц без дополнительного воздействия, но неясно, высока ли вероятность структурообразования и является ли процесс селиктивным. В статье представлена математическая модель, которая демонстрирует, как получить структуру из ансамбля частиц, описывает ее реализацию с помощью программного обеспечения и предлагает результаты вычислительных экспериментов.

Ключевые слова: математическая модель, самосборка наноструктур, вычислительный эксперимент, динамика Ланжевена.