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Metamorphosis of Dendritic Structures

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Abstract—A new way of modeling the self-organization of two-dimensional dendrites with randomly formed growth centers is proposed. Dendritic structures with different symmetries are obtained. The set of new original algorithms and programs allows a generalized analysis of the structure of dendrites and their fractal features.

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INTRODUCTION

The synergetic modeling of different biophysical processes, including those that comprise the stage of formation of nature-like dendritic nanostructures, is currently of great interest [1, 2]. Dendritic structures of this kind find application in biomedicine to treat and diagnose different diseases. Their properties can be used to study the origin of life on Earth and create new fractal antennas, sensors, nature-like systems and devices, and in other fields of science and engineering as well [3–6].

Despite the many studies [2–7] performed in this sphere, dynamic features of the formation of dendritic structures with stochastically formed growth centers and their limiting fractal characteristics remain poorly studied.

There is thus a need to develop new sets of algorithms and programs for synthesizing dendrites with growth centers that form spontaneously during the self-organization of dendrites that allow comprehensive analysis of their fractal features.

The aim of this work was to analyze the capabilities of models developed to describe qualitative changes in the distribution of particles constituting dendritic clusters at the initial stages of their formation.

DYNAMICS OF THE FORMATION OF DENDRITIC STRUCTURES

Programs for determining the spatial distributions of the particles using the properties of particle–cluster aggregation models are a convenient tool for modeling the growth of dendrites. A drawback that restricts potential applications of the familiar diffusion-limited aggregation (DLA) and ballistic aggregation (BA) algorithms and their multiple modifications [1, 2, 5, 7–10] is the difficulty of describing the stochastic autonomous formation of fractal growth centers. The new approach proposed by the authors for synthesizing dendritic clusters of an arbitrary symmetry with spontaneously formed growth centers is based on comprehensive use of the properties of the classical DLA and BA models which consider the interaction between the particles that make up a dendrite and the simultaneous motion of several particles. The computational scheme also includes establishing a quantitative criterion of the formation of a cluster's growth center. The software especially offers the possibility of switching to the classical DLA and BA models with preset growth centers [5, 9].

In the first step of the new algorithm, the random motion of particles in the working field is established. The paths of the motions are set in a way similar to that of the DLA and BA models [9, 10]. In Fig. 1a, sections of the path of a moving particle are shown prior to its attachment to the forming dendrite. Particles that move along random paths (the DLA model) at distance R_f from the newly formed dendrite begin to move rectilinearly (the BA model) toward the latter and become immovable upon touching it.

In the second step, a grid representation of the data is produced to optimize the growth rate of the dendritic structures. The grid divides the working domain into sectors where information on the particles present in the latter is stored (Fig. 1b). To increase the efficiency of the algorithm, we introduce effective radius R_{int} of particle interaction. Exceeding it makes this interaction negligible: $R_{int} < L$, where L is the size of the grid set so that each particle interacts only with others from its own cell and eight neighboring cells. The interaction of the particles is considered to be

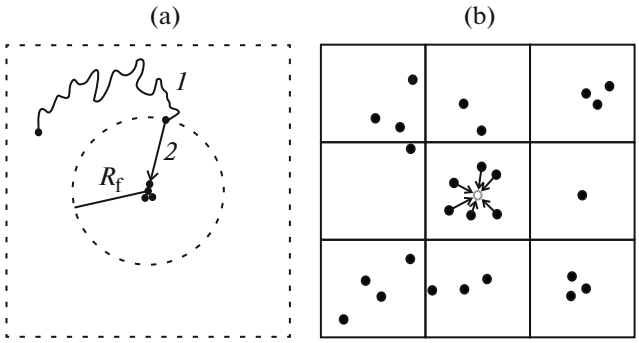

Fig. 1. Key fragments of the algorithm of dendrite growth: (a) sections of potential paths of the particles: (*1*) diffusion-limited aggregation model and (*2*) ballistic aggregation model (the dashed line marks the boundary of the working field) and (b) computational grid with particles (the arrows indicate the nucleation of new centers).

inversely proportional to the squared distance between them.

The arrows in Fig. 1b show a potential variant of the formation of a new dendrite growth center. Number N_{cr} of the particles in a grid cell is introduced as a quantitative parameter. When this number is achieved, the particles inside the relevant cell are replaced with a new dendrite growth center. In the central cell in Fig. 1b, we then have $N_{cr} = 6$. Note that the error introduced by omitting part of the particles from consideration is negligible for fractal dendrites with number of N of particles greater than 1000.

When in motion, the particles interacting with one another gather randomly in a finite space and form a new fractal cluster. Figure 2 shows the results obtained using the model developed for synthesizing different 2D dendritic structures with randomly formed growth centers. Figure 2a presents a variant of the model that is close to classical ones of centrally symmetric dendritic structures [2, 5, 7–10]. Number N of the particles that comprise the dendritic structure is 12000. The new program makes it unnecessary to establish a fixed growth center and calculate a random angle that characterizes the direction of the particle's path [10, 11]. During the calculations, a new particle was produced at a preset probability at every iteration in every peripheral cell, provided that it contained no immobile particles. If the particle traveled beyond the boundaries of the working field, it was excluded from consideration. To enhance the efficiency of the algorithm, modeling began in a small grid. This resulted in the formation of the first fractal cluster approximately in the center of the domain to be modeled. At the moment when all peripheral cells contained at least one immobile particle, the size of the grid was increased and calculations were repeated for the set of peripheral cells.

At the initial moment in time, particles were produced with probability P_b in every cell of grid N_b As they interact, they can form dendrite-like clusters that grow using only the starting material. Figure 2b shows a dendritic structure that formed according to the primordial soup model first proposed by Academician A.I. Oparin to describe the origin of life on Earth. During the formation of clusters, a branched dendritic structure of polymeric type was created that spread over the computational domain. Such a structure can

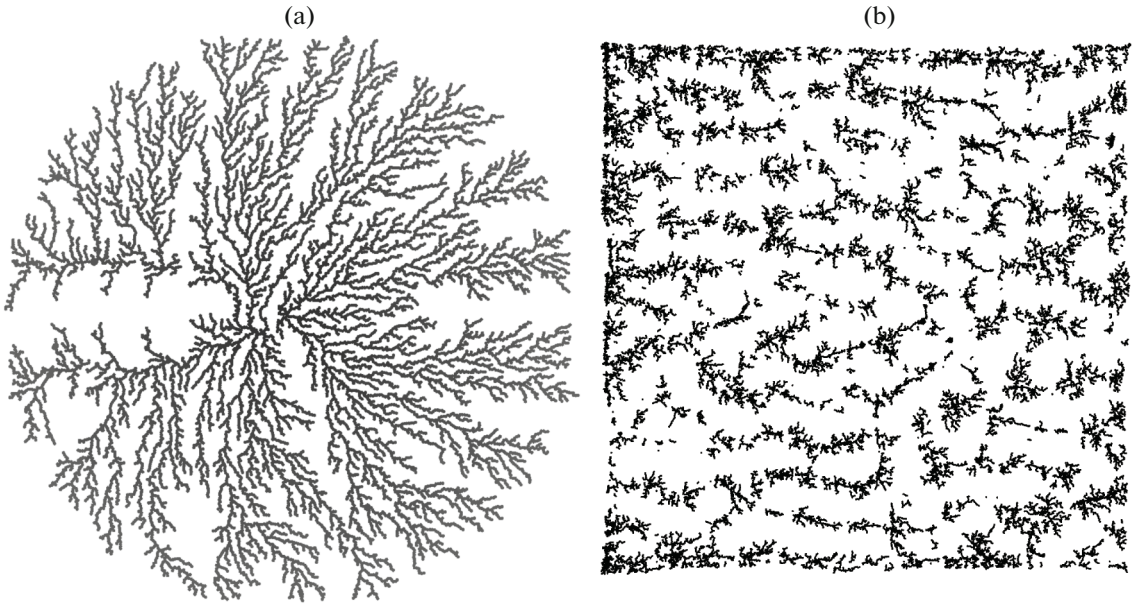

Fig. 2. Examples of modeling dendritic structures: (a) diffusion-limited aggregation model and (b) primordial soup model.

be used in materials science to synthesize and analyze new properties of polymeric dendrites [12].

FRACTAL RPOPERTIES OF DENDRITIC STRUCTURES

Fractal features of dendritic structures are conventionally estimated using tools of fractal parameterization [8, 13]. The key parameter is the fractal dimension. Different ways of calculating the fractal dimension (e.g., the similarity dimension, the box-counting (Minkowski) dimension, the correlation dimension, and the cluster (mass) dimension) are often used in the literature [8, 14]. This is normally due to specific features of a given object.

Our package of new original programs allows a generalized analysis of the geometry of dendrites and their fractal features. It is based predominantly on the mass and box-counting tools for determining fractal dimensions [8, 11].

The reliability of determining the fractal dimensions according to the above procedures was verified using simple test objects. The test objects were circles with a uniform and a nonuniform distribution of particles. With a uniform spatial distribution of the particles over a circle, the box-counting D_b and mass D fractal dimensions of the structures that formed were $D_b \approx D \to 2$ when number N of particles tended to 10^6. These estimates of the fractal dimensions served as a reference in the BA particle association model in [1]. The nonuniform distribution of the particles allows us to obtain different fractal dimensions by varying the looseness of the formed circle: $D_b, D < 2$. Such test estimates of fractal dimensions correspond to the 2D DLA model.

The results from modeling the formation of 2D fractal dendritic structures (Fig. 2) in different ways show that the limiting averaged fractal dimension of centrally symmetric dendritic clusters is close to $D \approx D_b = 1.71$ when number N of particles tends to 10^6.

We have therefore established the dynamics of changes in the fractal dimensions of individual clusters with different symmetries, depending on the number of the constituent particles.

CONCLUSIONS

The proposed computation scheme for the formation of dendritic structures with randomly formed growth centers is a valuable alternative to the particle–cluster aggregation models used earlier. It allows us to synthesize fractal dendritic clusters of various geometries, different degrees of sparsity, and different positions simply by setting the required input parameters. Our model offers new possibilities for the targeted growth of dendrites with random growth centers that can be used to model the morphogenesis of different biological objects.

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