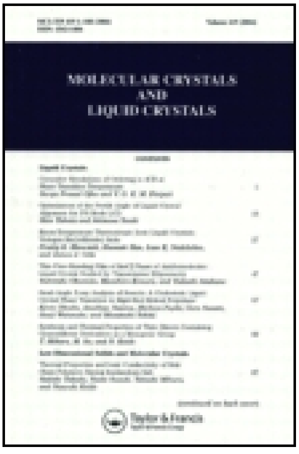

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Local Structure Analysis of Diffusion-Limited Aggregation Clusters

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Some morphometrical characteristics for quantitative DLA-structures description are proposed. They can reliably distinguish DLA-clusters, which have different structures on short length scale.

1. INTRODUCTION

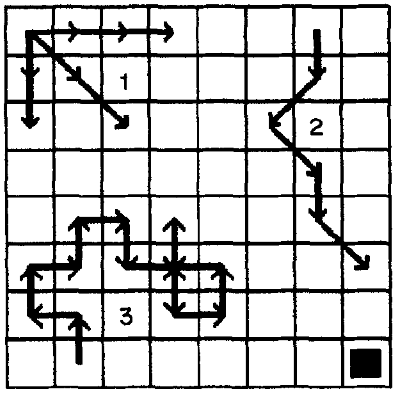
The diffusion-limited models studying the aggregation processes in crystal and biological growth are important both in scientific and practical aspects. Recently, a strong recurgence of interest in development of better understanding of non-equilibrium growth and aggregation processes has occurred. Many extensions of DLA-models [1–3] have been developed to investigate the effects of plausible physical processes such as reorganization during or after aggregation, rotational diffusion, spatially homogeneous or concentric particle drift on DLA patterns. In most cases, such modifications have little or no effect on the fractal dimension but may drastically modify the structures on short length scale.

From the above-mentioned aspects, let us here examine the correlations of DLA-cluster structure on short length scale and some their morphometrical parameters to reach reliable conclusions concerning a quantitative description of the simulated patterns. The present model and morphometrical parameters will be described in Sections 2 and 3 respectively. Finally Section 4 addresses some discussions and conclusions.

2. MODEL

Let us begin with the explanation of the present simulation model. In this work, we shall restrict our model to a two-dimensional square lattice 256 × 256 points. First of all, let us define two types of our model.

In the first model type the growth process starts with a single stationary particle and other particles are added, one after another, to a growing cluster (or aggregate) of particles. Particles can follow random ballistic (linear) or "broken" or Brownian (diffusion) trajectories in the vicinity of the seed particle (Figure 1a).



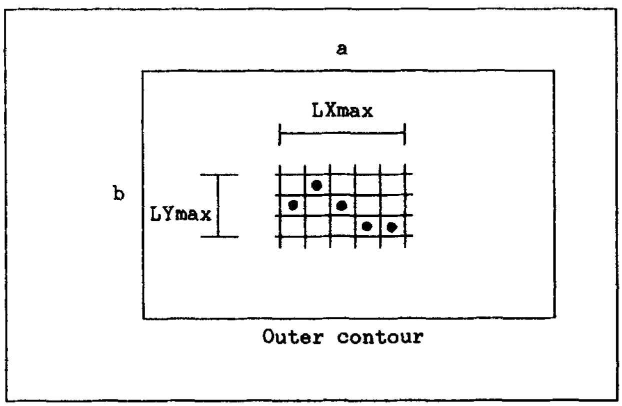


FIGURE 1 (a) Particles' trajectories examples. ■ the seed particle. 1, "ballistic", 2, "broken", 3, "diffusion" particle trajectories. (b) Outer contour size and position, $a = \text{LXmax} + \Delta 1$, $b = \text{LYmax} + \Delta 1$.

In the second model type particles density (C) is constant, i.e., initial model configuration is a population of particles set on lattice sites randomly. The growth process starts with the seed particle in the lattice center too. But the particles trajectories are only linear ("billiard balls") or Brownian (diffusion). We shall call these model kinds "Walk-ballistic", "walk-broken", "walk-diffusion", "density-linear" and "density-diffusion", respectively.

The displacement rule of moving particle in the first model type is assumed to be

$$\Delta x = f_x, \quad (1)$$

$$\Delta y = f_y,$$

where Δx and Δy are the relative displacement components along x and y axes, respectively, f_x and f_y are the fluctuation forces, which are choosen from sequence $-1, 0, 1$ randomly. But random choice must be such that moving particle flights towards the seed particle. Direction of moving particle is defined by its original position in regard the seed particle. Examples of particles trajectories are given on the Figure 1a. To erase a particle randomly walking outwards the size of outer contour (see Figure 1b) is set to

$$a = LX\max + \Delta 1 \qquad (2)$$

$$b = LY\max + \Delta 1,$$

where $LX\max$ and $LY\max$ are the maximum projections of the growing cluster on the x and y axes respectively. As soon as the moving particle goes out of the outer contour, then a new moving particle is set in a random point of the outer contour.

The second model type is based on the cellular automata logic [4], so the displacement rule of moving particle is points transposition rule in four-points Margolus-neighbourhood of lattice.

For both model types randomly walking particle is eventually stuck on the growing cluster as it arrives at an active site adjacent to the cluster. We use two masks of active sites, i.e., two sticking conditions. If moving particle arrives at one of 4 or 8 (Figure 2a)

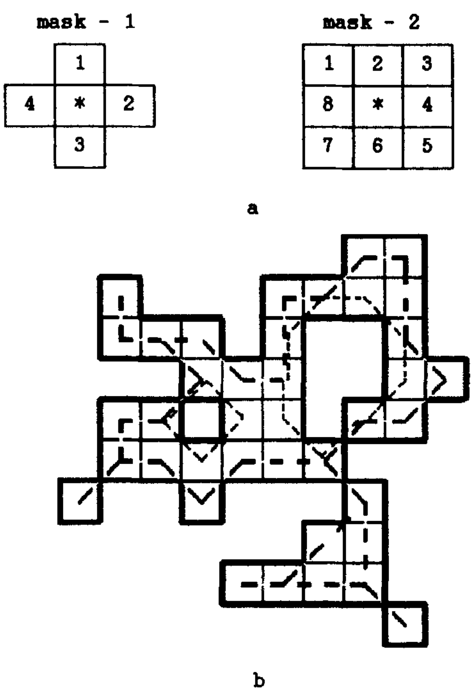


FIGURE 2 (a) Two masks of active sites. (*) Site belongs to cluster. (b) Morphometric parameters. ■■■ external perimeter, $P1$, ------ internal perimeters, $P2$ and $P3$. $S1$, $S2$, $S3$ are the squares compassed by $P1$, $P2$, $P3$ perimeters respectively. Pext $= P1$, Sext $= S1$, Psum $= P1 + P2 + P3$, Ssum $= S1 - S2 - S3$.

TABLE I

Present Model Kinds

Type	Trajectories	Sticking condition mask	Model kind
I	"Ballistic"	8 points	"Walk-ballistic"
	"Broken"	8 points	"Walk-broken"
"Walk"	"Diffusion"	8 points	"Walk-diffution-8"
		4 points	"Walk-diffution-4"
II	"Linear"	8 points	"Density-linear"
"Density"	"Diffusion"	8 points	"Density-diffution-8"
		4 points	"Density-diffution-4"

neighbouring sites of the particle, which belongs to the cluster, it sticks to the cluster. Both sticking conditions are used for diffusion paticles' trajectories and the first condition is only used for "ballistic", "broken" and "linear" particles' trajectories.

Thus, seven model kinds, which will be below investigated, are shown in the Table 1.

3. MORPHOMETRIC PARAMETERS

Let us take into account following morphometrical parameters:

1. Number of particles in the cluster (Psum).
2. Number of bound particles in the cluster (Pbnd), which is defined according to the mask-1 shown on Figure 2a. If one of four neighbouring sites adjacent to the cluster particle is empty, this cluster particle is bound particle.
3. Length of the whole cluster perimeter (Lsum).
4. Square of cluster (Ssum).
5. Length of the external cluster perimeter (Lext).
6. "External" square of cluster (Sext).
7. Mean Feret diameter of cluster $\overline{DF}$.

Perimeter length and cluster square are calculated as chain code (or Freeman code) round of cluster contours is carred out [5] (Figure 2b).

Feret diameter is the largest cluster projection on certain direction (Q) [6–8]. The mean Feret diameter is

$$\overline{DF} = (1/\pi)\int_0^{\pi} Df(Q)\,dQ.$$

We calculate DF as mean value of twenty Feret diameters for directions from 0 ° to 171° with step 9°.

Fractal cluster dimension D will be evaluated using function [9, 10]

$$\text{Psum} = \overline{DF}^{D}. \tag{3}$$

Let us assume correlation between following parameters

$$\begin{aligned} \text{Psum} &= f_1(\text{Pbnd}), \\ \text{Lsum} &= f_2(\text{Ssum}), \\ \text{Lext} &= f_3(\text{Sext}). \end{aligned} \quad (4)$$

The purpose of the next section is investigation of the cluster local geometry effects on these characteristics.

4. SIMULATION RESULTS AND DISCUSSION

For each model kind ten experiments were carried out, when the control parameter ($\Delta 1$ and C for the first and the second model type, respectively) was fixed and fractal patterns for each of 10 experiments were statistically similar. So the simulation results for each characteristic are

$$x = x \pm \Delta x,$$

where x is a mean value of characteristic and x is a standart error calculated from results of ten computer experiments.

First of all, let us examine the f_1, f_2, f_3 curves shape. It appears that these curves are linear for all model kinds (Figure 3). Consequently, Equations (4) can be approximately defined as

$$\text{Pbnd} = k1 \cdot \text{Psum}, \quad (5)$$

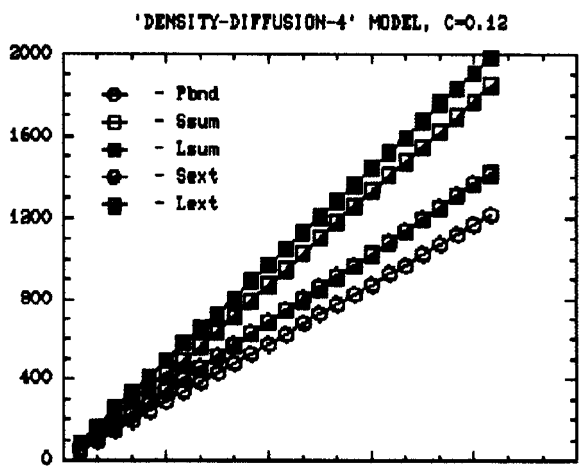


FIGURE 3 "Density-diffusion-4" model, $C = 0.12$. N is particles' number in cluster.

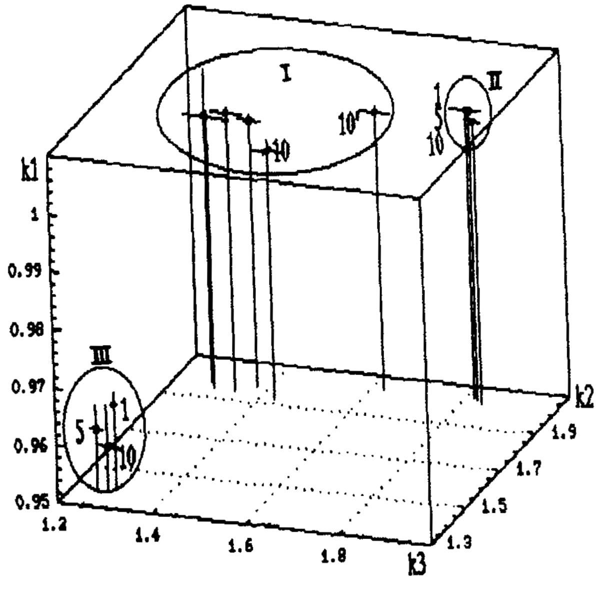


FIGURE 4 (I) "walk-ballistic" and "walk-broken" models (10)- "walk-balistic" model), (II) "walk-diffusion-8" model, (III) "walk-diffusion-4" model. Numbers are the values Δ1 for each model kind.

$$\text{Lsum} = k2 \cdot \text{Ssum},$$

$$\text{Lext} = k3 \cdot \text{Sext}.$$

Thus, coefficients $k1, k2, k3$ are the universal characteristics of fractal structures because $k1$, $k2$, $k3$ do not depend on cluster size and linearity of the $f1, f2, f3$ confirms self-similarity, or size invariance, of the fractal structures. Let us describe these characteristics as follows

- $k1$ presents "inverse cluster branch thickness" or extent of cluster loose packing. $k1$ is 1 for the cluster, in which each particle is a bound particle.
- $k2$ defines cluster ability to form close contours (or cavities for three-dimension case).
- $k3$ characterize branching of external cluster contour.

Hence, we shall below analyse simulation clusters using these morphometrical characteristics.

Quantitative images of clusters generated by the first model type are presented on Figure 4. Three cluster groups can be clearly seen on the parametric planes $k1$–$k3$ or $k2$–$k3$, and two cluster groups—on the plane $k1$–$k2$. Three distinct cluster groups correspond to their visual forms (Figure 5a–d). So changing 4-points active sites mask to 8-points mask in "walk-diffusion" model results in more crumbly structure. This structure modification on short length scales is clearly distinguished in plane $k2$–$k3$. Cluster structures generated by "walk-ballistic" and "walk-broken" models are little

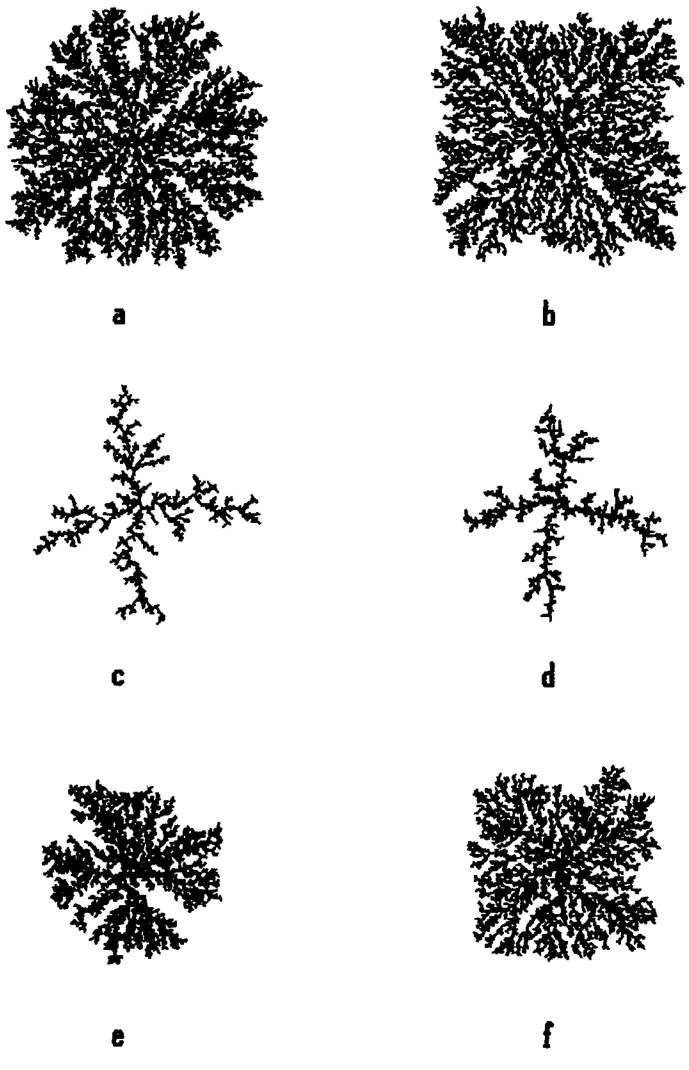


FIGURE 5 Simulation clusters. $\Delta 1 = 5$: (a) "walk-ballistic", (b) "walk-broken", (c) "walk-diffusion-8", (d) "walk-diffusion-4"; $\Delta 1 = 10$: (e) "walk-ballistic", (f) "walk-broken".

distinguished both visual and quantitatively. It has a simple explanation. "Ballistic" and "broken" particles' trajectories are small different on the short distance $\Delta 1$ ($\Delta 1 = 1$ and $\Delta 1 = 5$) and more different on the distance $\Delta 1 = 10$ (Figure 5e, f).

For the second model type we investigated evolution of morphometrical characteristics as particles' density C increases. Dependence D vs. C for all three cases (Figure 6a) is linear, i.e., fractal dimension does not characterize structure modifications as C increases. In this case, the most informative characteristic is $k3$ (Figure 6b). It can be clear seen critical value Cc on the plot $k2$ vs. C for the "density-diffusion-4" and "density-diffusion-8" models. This critical point correspond to the phase transition because of the formation of many close contours or cluster branches lincking (Figure 7a–d).

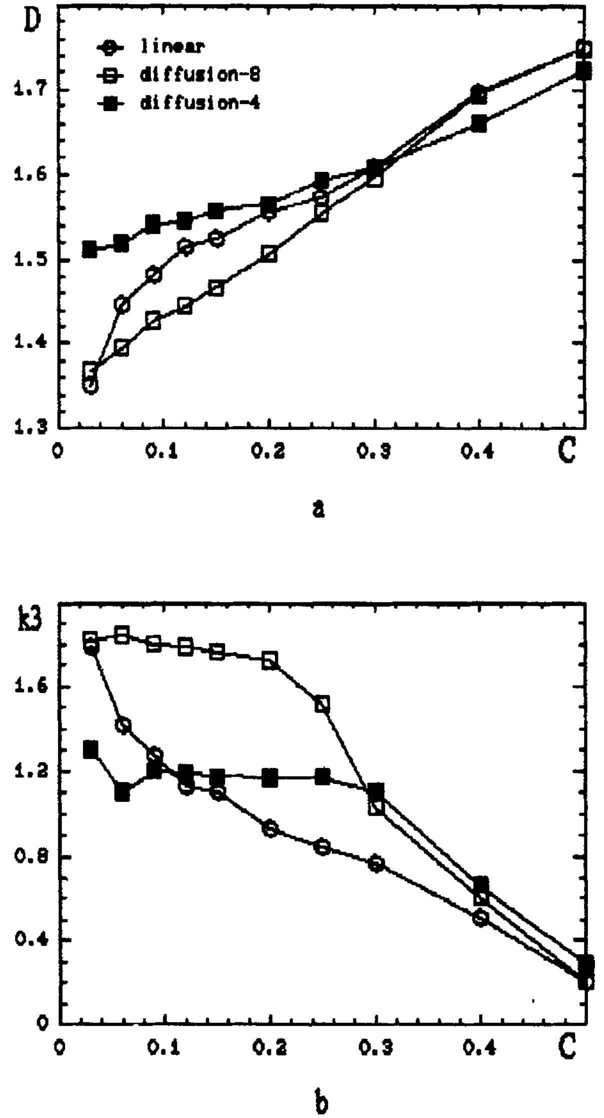


FIGURE 6 (a) plots "Fractal dimension vs. particle density". (b) plots "$k3$ vs. particle density" for the second model type. $Cc = 0.2$ for "density-diffusion-8" model, $Cc = 0.03$ for "density-diffusion-4" model.

Increasing of C value above Cc leads to the percolation cluster. There is no such critical value for "density-linear" model because close contours are formed for all C values (Figure 7e, f). This special feature is intrinsic for "linear" particles' trajectories.

In conclusion, it should be noted that the morphometrical characteristics proposed in this work can be used for recognition of real fractal structures using computer systems of image analysis.

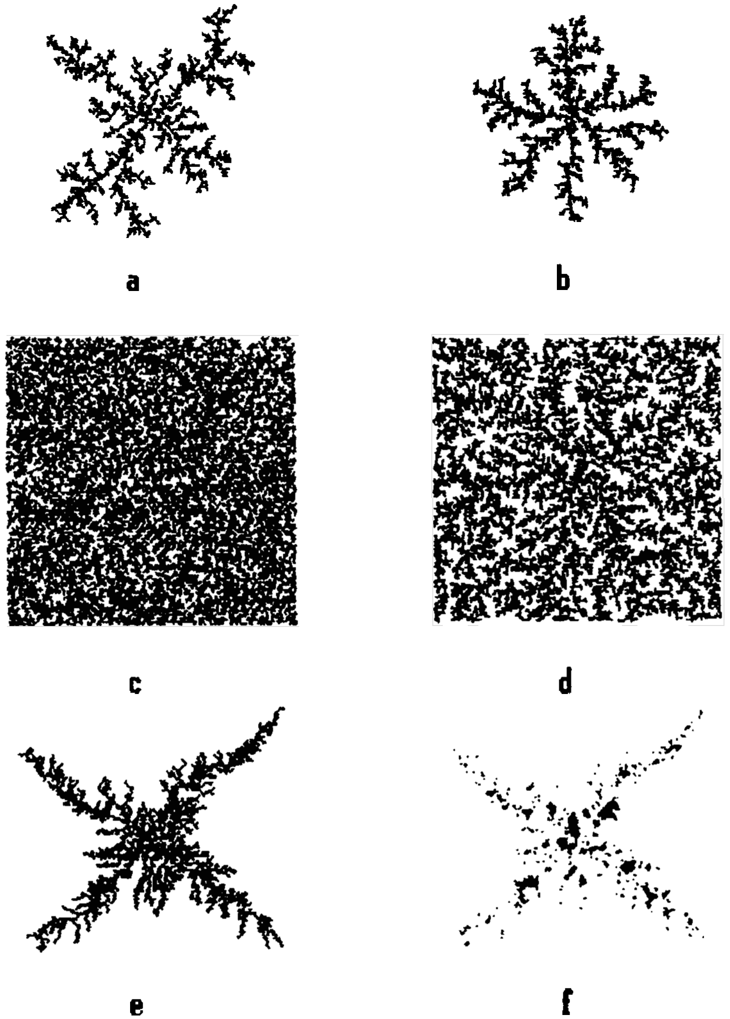


FIGURE 7 Simulation clusters. (a, b) $C = 0.03$, "density-diffusion-8" and "density- diffusion-4" respectively. (c, d) $C = 0.30$, "density-diffusion-8" and "density-diffusion-4" respectively. (e, f) $C = 0.06$, "density-linear" model, (e) clusters, (f) flooded close contours of this cluster.

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