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INTERFACE STRUCTURE IN COLORED DLA MODEL

V.Tchijov, S.Nechaev, S.Rodriguez-Romo*

Centro de Investigaciones Teoricas, Universidad Nacional Autónoma de México, Campus Cuautitlán, Cuautitlán Izcalli, Edo. de México, 54768 México

**L.D.Landau Institute for Theoretical Physics 117940, Moscow, Russia*

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We propose a model for the simultaneous diffusion-limited growth of two clusters *A*- and *B*-, where the growth of one cluster screens the growth of the other one. We consider the possibility that the *A* and *B* clusters can penetrate into each other in course of their growth in different spatial dimensions and express the conjecture that the *A*–*B* boundary is flat in all dimensions. Using an electrostatic analogy, we compute some spatial characteristics of the clusters.

Introduction. Since 1981, when Witten and Sander [1] invented the model of diffusion-limited aggregation (DLA), interest in the investigation of the statistical properties of DLA clusters has remained very great. The reasons for such steady attention to various aspects of DLA models is accounted for by the following facts: (i) DLA clusters have very unusual fractal properties, exhibiting a dependence of the fractal dimension on the cluster size (i.e., so-called multifractal behavior); (ii) DLA models have valuable physical applications for describing such phenomena as breakdown in dielectric materials, the growth of "viscous fingers" in liquids, and so on (see [2] for a review).

Despite essential success in describing the fractal properties of DLA clusters, models of diffusion-limited aggregation appear to be not so simple for theoretical investigations. In particular, conformal methods and the renormalization group approach need some modifications on account of the forementioned multifractality. Thus until now numerical simulations have remained the most reliable methods for treating DLA. The many papers devoted to numerical analysis of different modifications of the DLA model give rather comprehensive information about the "zoology" of these fractal objects. At the same time the interactions of immobile DLA clusters have received much less attention in the literature.

In the present work we propose a model for the interaction of two immobile DLA clusters and pay particular attention to the structure of the interface between these clusters. Namely, we examine whether DLA clusters can penetrate into each other during their growth in different spatial dimensions. Let us mention also that the model proposed in the present work establishes a bridge between two different problems: diffusion-limited aggregation, and random walks in systems with distributed (non-point-like) traps.

Model and Numerical Simulations. We formulate the model in a D-dimensional space. Suppose we have two particles of two different kinds (colors) A and B, which we place on a D-dimensional cubic lattice at a distance d from each other (d is measured in units of the lattice spacing). These particles serve as the initial (generating) points of A and B clusters.

Suppose that on the surface of a D-dimensional sphere S of radius R_D ($R_D \gg d$), the center of which is placed at the midpoint of the segment connecting the initial A and B particles, we create, at a random point, particles A or B independently with equal probabilities. The interaction between particles is defined as follows (see Fig.1):

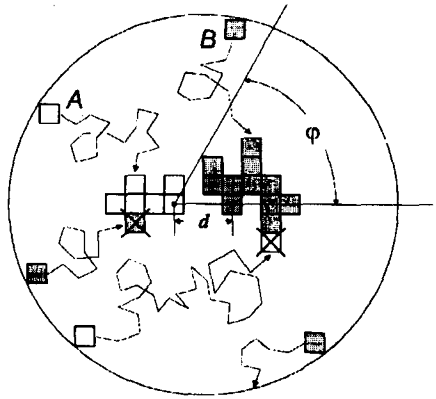

Fig.1. (a) Schematic model of "colored" diffusion limited aggregation

1. If a randomly moving particle with color A (B) reaches a lattice point neighboring to the initial (generating) particle A (B), then the diffusing particle sticks to the initial particle to form a new initial cluster of two A (B) particles.

2. If a randomly moving particle with color A (B) reaches a point neighboring to the initial cluster of particles B (A), then this diffusing particle disappears ("dies"). If some lattice point is a common neighbor for both growing clusters A and B, then any diffusing particle dies when reaching this point.

The question of our main interest concerns the structure of the interface separating the growing A and B clusters. *A priori* the following situations could be realized in the system under consideration: (i). For $D \geq 2$ the growing clusters A and B penetrate each other by the branches, so that an interface does not actually exist; (ii) spontaneous symmetry breaking occurs in the system, resulting in the complete supression of the growth of one cluster by the other one; (iii) clusters A and B grow in such a way that they do not penetrate each other deeply. Of course, different structures among those described could be realized in different dimensions.

The results of numerical simulations of the growth of A and B clusters interacting according the rules proposed above are shown in Figs. 2–3, where the most typical structures are shown for $D = 2, 3$ and two different distances between initial (generating) particles: $d = 2, 100$. It can be seen that the A and B clusters are non-interpenetrating. Below we adduce some theoretical conjectures in support of the hypothesis that A and B clusters do not penetrate each other in any dimensions and remain completely separated.

Let us mention briefly some technical details relevant to the numerical simulations of the described model. We used the modification of the original method of Witten and Sander proposed and utilized by Meakin [1]. We put a particle A or B (the color of the particle is chosen randomly) at a random point of a d-dimensional sphere S, the radius of which, R_D, grows dynamically with the formation of the cluster. The particle then diffuses on a d-dimensional cubic lattice. If the particle escapes the system, i.e., reaches some point which is located at a distance of three times the maximum cluster radius, R_{max}, it is killed and a new particle is created.

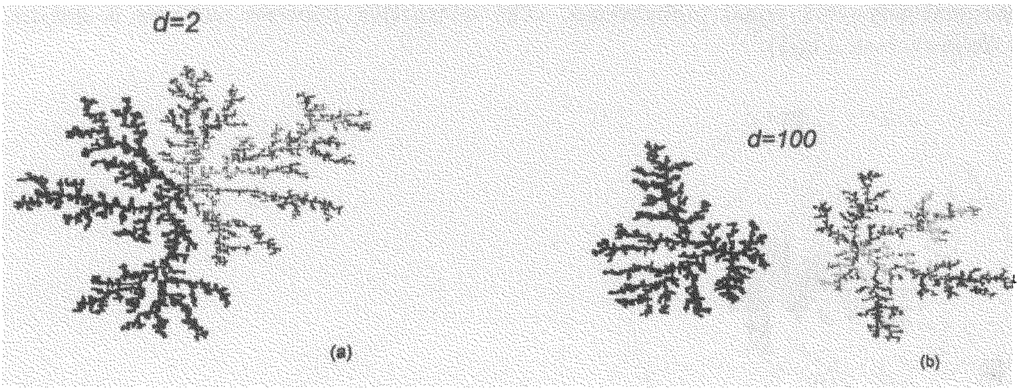

Fig.2. Typical 2D-realisation of *A–B* cluster growth ("time series") for $d = 2, 100$

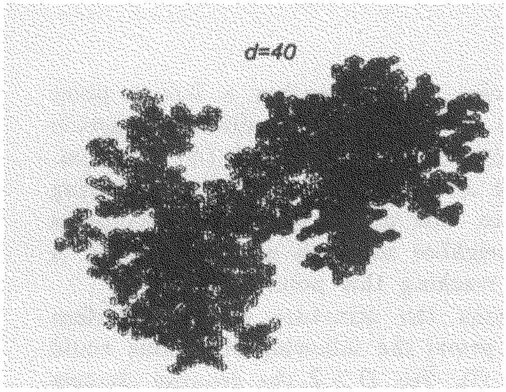

Fig.3. Typical 3D-realisation of *A–B* cluster growth ("time series") for $d = 40$

When the particle reaches one of the clusters, it attaches or "dies" in accordance with the algorithm described above. To reduce the required computer time and speed up the calculations we multiplied the elementary step of the diffusing particle by a factor of 2, 4, 8, etc. if the particle was at distances of $R_{\max}+10$, $R_{\max}+20$, $R_{\max}+40$, etc. from the origin [1]. A comprehensive investigation of the described method of particle generation for the standard diffusion-controlled cluster formation has been presented recently by Voss [2]. To produce the random choice of color, initial position of the particle on the *d*-dimensional sphere, and direction of motion of the particle we utilised the random number generator RAN3 described in [3]. In order to accelerate the procedure of checking the contact of a moving particle with already existing clusters we used the method of so-called hash-coding with linear probing as a collision-resolution scheme [4, 5]. Our programs were written in Borland Pascal and run on a 60 MHz Pentium system. Because of computer limitations we generated clusters of moderate sizes of up to 3000 particles in the largest cluster.

Discussion. 1. We believe that the fact of the mutual impenetrability of *A* and *B* clusters is accounted for by two facts: (i) the absence of an upper critical dimension in the DLA model, and (ii) the "spontaneous symmetry breaking" (or fluctuational instability) in the initial stages of cluster growth.

Recall that in the 2D case the fractal dimension $D_{\rm DLA}$ of the ordinary DLA cluster lies in the interval $1.5 < D_{\rm DLA} < 1.75$ [8] and in higher dimensions ($D \gg 1$) $D_{\rm DLA} \to D-1$ ($D_{\rm DLA} < D-1$) [9].

The absence of an upper critical dimension means that the DLA cluster will grow almost completely fillng the free space on the lattice. Actually, the cluster density ρ can be estimated as $\rho \sim N/R^D$, where N is the number of particles in the cluster and R is its size ($R \sim N^{1/D_{\rm DLA}}$). Thus we have $\rho \sim N^{-1/(D-1)} \to 1$ for $D \gg 1$. Hence, if at some moment of time a part of the space is occupied by the A cluster, then the growth of the B cluster in this part of space is completely screened. In other words, the large-scale behavior of cluster growth is determined by the fluctuations of diffusing particles and screening in the initial stages of growth.

Let us mention that the same conclusion concerning the penetration depth can be obtained if we consider the A–B colored aggregation from the point of view of statistics of diffusion-controlled reactions on fractals, i.e., if we regard the DLA cluster (say, A) as a "distributed trap" for diffusing particles B. It means that we forget about the specific structure of the cluster A and, in the volume occupied by the cluster, put in "traps" with a mean concentration

$$\rho = \frac{N}{R^D} \sim N^{1-D/D_{\rm DLA}}. \tag{1}$$

The particles B diffuse freely and penetrate the volume V containing the traps. In the mean-field Smolukhovski-type approach we have the following expression for the concentration $C(t)$ of particles B in the volume V at time t (see [10] for a review):

$$\frac{C(t)}{C(0)} = \exp\left(-\rho \int_0^t dt'\, K_{\rm Smol}(N,t)\right), \tag{2}$$

where the reaction constant $K_{\rm Smol}(N,t)$ has the following asymptotic behavior [11]

$$K_{\rm Smol}(N,t)\Big|_{t\to\infty} \sim N^{1/D_{\rm DLA}}. \tag{3}$$

Substituting Eq.(3) into Eq.(2) we get

$$\frac{C(t)}{C(0)} \propto \exp\left(-N^{1-(D-1)/D_{\rm DLA}}\, t\right). \tag{4}$$

Thus the concentration of particles B diffusing in the volume V decreases exponentially with the time t. Using the obvious relation $R \sim a\,t^{1/2}$, we come to the conclusion that the DLA cluster is completely "non-transparent" for diffusing particles, which is consistent with the arguments presented above.

2. In order to have some quantitative estimates concerning the simultaneous growth of A and B clusters, let us generalize our model in the following way. We shall generate the particles of type A (B) with the probabilities $p_A \geq 1/2$ ($p_B = 1 - p_A$).

The structure of growing clusters resembles geometrically the structure of electric field lines of two oppositely charged particles. Thus the boundary between A and B clusters can be regarded as an equipotential surface. This analogy, supplemented by the statement that the A–B boundary is flat, can be used for calculation of the average angle inside which the smaller cluster is growing (see Fig.1).

We restrict discussion to the 2D case. In the framework of the electrostatic analogy it is easy to write the 2D potential $\Psi(\mathbf{r})$ created at the point $\mathbf{r}$ by two charges $q_A > 0$ and $-q_B$:

$$\Psi(\mathbf{r}) = q_A \ln \frac{|\mathbf{r}|}{\tilde{a}} - q_B \ln \frac{|\mathbf{r} - \mathbf{r}_{AB}|}{\tilde{a}}, \tag{5}$$

where $|\mathbf{r}_{AB}| = d$, while $\tilde{a}$ is regarded as a free parameter which we choose from a comparison of the numerical data with analytical results. Let us stress that $\tilde{a}$ has the meaning of the "effective lattice cell" and has not yet been specified. In the polar coordinates (ρ, φ) we have

$$\Psi(\mathbf{r}) = q_A \ln \frac{\rho}{\tilde{a}} - q_B \ln \frac{\sqrt{\rho^2 + d^2 - 2\rho d \cos\varphi}}{\tilde{a}}. \tag{6}$$

The equipotential surface $\Psi(\mathbf{r}) = 0$ is determined by the equation

$$\beta = \frac{\ln \sqrt{\rho^2/\tilde{a}^2 + d^2/\tilde{a}^2 - 2(\rho d \cos\varphi)/\tilde{a}^2}}{\ln \rho/\tilde{a}}, \tag{7}$$

where $\beta = q_A/q_B$. It is very natural to associate the value of β with the fraction $p_B/(1 - p_B)$ $(p_B < 1/2)$.

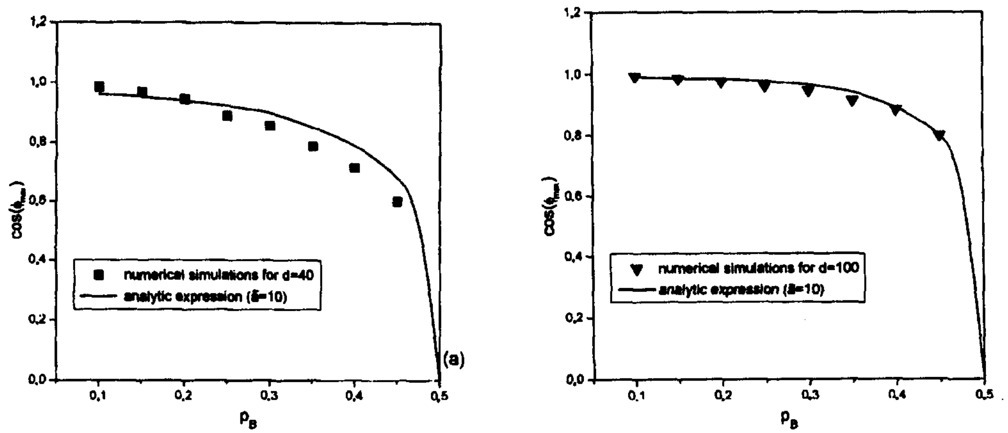

Fig.4. Plot of the function $\cos\varphi_{max}(p_B)$ (2D-case). The solid line shows analytical results ($\tilde{a} = 10$); the squares (a) and triangles (b) represent the averaged data of numerical simulations for distances $d = 40$ and $d = 100$, respectively

To find the maximum value of the angle $\varphi_{\max}$ inside which the cluster B is growing, we have to minimize the equation for $\cos\varphi$,

$$\cos\varphi = \frac{(\rho/\tilde{a})^2 + (d/\tilde{a})^2 - (\rho/\tilde{a})^{2\beta}}{2(\rho d/\tilde{a}^2)}, \tag{8}$$

with respect to ρ.

A plot of the function $\cos\varphi_{\max}(p_B)$ together with the averaged value $\langle\cos\varphi_{\max}(p_B)\rangle$ obtained from the results of the numerical simulations (for the

2D model) is presented in Fig. 4a, b for $d = 40$ and $d = 100$. The averaging is performed over 100–150 realisations of the clusters (or "time series") for each value of p_B. The effective lattice spacing $\tilde{a}$ is the same in both cases, $\tilde{a} = 10$. It can be seen that the agreement of the analytical and numerical results is better for $d = 100$, a fact which we explain by the circumstance that the role of cluster size fluctuations in the initial stages of the cluster growth is a decreasing function of d.

The moderate sizes of clusters (3000 particles in the largest cluster) do not allow us to obtain reliable results for $p_B = 1/2 - \epsilon$ ($|\epsilon| \ll 1$), i.e., when $\cos\varphi_{max} \to 0$ ($\varphi_{max} \to \pi/2$).

The extention of the above "electrostatic analogy" to higher dimensions is planned for a separate publication. If our conjecture is true, we can expect that the value of the angle φ_{max} will not depend on d, because the corresponding electrostatic potential has power-law (and not logarithmic, as in the 2D case) behavior.

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