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Diffusion limited aggregation of particles with different sizes: Fractal dimension change by anisotropic growth

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ABSTRACT

Clusters formation models have been extensively studied in literature, and one of the main task of this research area is the analysis of the particle aggregation processes. Some work support that the main characteristics of this processes are strictly correlated to the cluster morphology, for example in DLA. It is expected that in the DLA clusters formation with particles containing different sizes the modification of the aggregation processes can be responsible for changes in the DLA morphology. The present article is going to analyze the formation of DLA clusters of particles with different sizes and show that the aggregates obtained by this approach generate an angle selection mechanism on dendritic growth that influences the shielding effect of the DLA edge and affect the fractal dimension of the clusters.

1. Introduction

It is well known in literature that growth phenomena as crystal formation and polymerization that have morphological structures with a great number of singularities, can be simulated using a Diffusion Limited Aggregation model (DLA). The DLA model proposed by Witten and Sander [1] in 1981, due to its simplicity on a computational perspective and morphological complexity exposed on the grown structures, remarks it as a useful tool to work with a huge number of modified models to represent from biological [2] and thin films [3] to crystal [4] structures.

Many statistical and geometrical features associated with DLA have been studied across the years. The fractal dimension [5], pair correlation functions [6] and other parameters are very well known. In general, the values of this properties are related to the main characteristics of the walk and the aggregation processes [7], for example, alterations on particle path turning them into biased walks [8–10]. These modified models try to reproduce some phenomenological behavior of certain systems, for example, the convection drift [11], an unusual drift produced by a force field [12] and different patterns formatted during crystallization processes [13].

Another important variable that plays an important role on the determination of some geometrical and statistical features associated with the cluster are the shape of aggregated particles. Real systems that can be modeled as DLA, generally do not present symmetric and identical particles, so in order to capture this realistic properties of inhomogeneity in the aggregated

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Table 1
Simulation parameters.

Symbol	Name
R_L	Launching radius
R_k	Killing radius
$R_{\max}$	DLA radius
r	Particle radius
r_m	Maximum particle radius

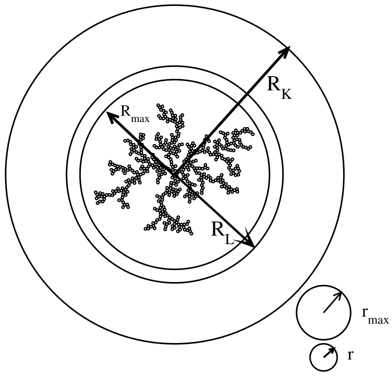

Fig. 1. Diagram of the main variables associated with the DLA model simulated. The name of each parameter can be obtained in Table 1.

particles morphology some research have been reported in literature [14]. The influence of *seed* particles with different sizes was evaluated on the study developed by Wu et al. [15]. Another approach taking into account not only the first particles aggregated was reported by Tan et al. [16] and DLA with particles with different geometrical shape was analyzed by Li et al. [17].

The correlation between the aggregation of particles with different sizes and the direct influence of it on the DLA morphology have not been shown in literature. Hence, our work is going to investigate qualitatively and quantitatively the connection between the particle dimensions and the fractal morphology of the DLA obtained by calculating their fractal dimension and three pair correlation functions, in special angular pair correlation function that is used to measure the angle selection mechanism associated with the dendritic growth.

2. Model

Our off-lattice DLA model was based on the algorithm proposed in Ref. [18]. The main parameters used on the simulations are listed in Table 1. As observed in Fig. 1, $R_{\max}$ is the DLA radius, defined as the distance between the *seed* (first particle aggregated) and the farthest particle aggregated with respect to the *seed*. The killing radius R_k is a limiting circle used to identify a disposal event when the walking particle cross that line, so that another particle is released at an aleatory point on the circle of radius R_L. Before the particle begin the random walk, it is attributed a value of radius for it in the range $0 \leq r \leq r_{\max}$, where $r_{\max}$ is an external parameter specifically chosen for each simulation representing the maximum radius that any particle can have.

The aggregation tests evaluated, and the rearranging tests for the cases of particles superposition are the same proposed in Ref. [18].

In order to morphologically characterize the aggregates the fractal dimension using the mass–radius calculation similar to the one of Ref. [5] was performed. To determine a possible mechanism of angle selection in the dendritic growth the angular pair correlation function $\tilde{C}(\theta)$ was evaluated, and to analyze the homogeneity of the DLA a typical pair correlation function $\tilde{C}(R)$ was performed [5,6].

After the DLA cluster was obtained, we calculate the average distribution number $n = \langle N_i/N_{total}\rangle$ of particle with radius r_i to analyze the population of each kind of particle.

The mass–radius calculation was performed counting the number $N(r)$ of particles inside a circle of radius r and centered on the *seed*. To take into account the particles with different sizes, along the calculations of $N(r)$ each particle was weighted with a factor r_i^2. The Dilogarithm graphic of $\log(N(r)) \times \log(r)$ presents a region with a power law relation $N(r) \propto r^{D_f}$ where D_f is the fractal dimension of the DLA [5].

The pair correlation function $C(R)$ was calculated as

$$C(R) = \sum_{i=1}^{N}\sum_{j=1}^{N}\delta(R_{ij}) \quad (1)$$