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SHORT COMMUNICATION

M.G. Bertoluzzo
S.M. Bertoluzzo
J.A. Luisetti
C.A. Gatti

A bidimensional simulation of particle-cluster aggregation with variable active sites particles

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M.G. Bertoluzzo (✉) · S.M. Bertoluzzo
J.A. Luisetti · C.A. Gatti
Facultad de Ciencias Bioquimicas
Y Farmaceuticas
Departamento de Quimica-Fisica
Suipacha 531
2000 Rosario
Argentina

Abstract In this work a simple program has been developed which simulates the process of particle–cluster aggregation limited by diffusion. All the simulation have been carried out using 2d square lattices with square "particles" having a variable number of active interaction sites (from 3 to 8) for each particle in order to analyze the effect of such limitation on the fractal dimension of the aggregates. The fractal dimension of such aggregates was calculated by the so-called "box counting" method. It has been shown that there is no change in the value of the fractal dimension (1.70) as the active site number is increased. Instead it appears that there is an average number of active sites of about 2.3 for all the structures no matter how many active interaction sites the particles have. This appears as an interesting result in connection with the aggregation of particles such as renneted casein micelles, which could present differences in the surface density of active sites.

Key words DLA – simulation – colloidal aggregation – active sites – fractal dimension

Introduction

The process of aggregation or flocculation of small particles to form larger clusters and the structures that result are technologically and scientifically important. Virtually, all of our knowledge of the growth of these structures has come from computer simulations, which have suggested that the resultant structures exhibit scale invariance and can be well described as fractals.

In recent years, a considerable interest in particles aggregation models which simulate processes like colloidal aggregation, dendritic growth, biological growth, etc., has been developed. This interest was stimulated by the development of the diffusion limited aggregation (DLA) model introduced a few years ago by Witten and Sanders [1], and because of the recognition that these models and others very close to it [2, 3], conduct to the formation of structures with a characteristic fractal dimension (D) less than the one of the space or lattice (d) in which the aggregation is occurring. Since the physics of fractal growth lacks a unified theoretical description, these models give a base to improve the comprehension of many real processes of growth and aggregation [4]. In this work, a DLA model taking into account the possibility of varying the number of the active sites on the particle surface was introduced. The influence of such variation on the fractal dimension was analyzed.

Simulation in a square lattice

Rules of the model: A seed particle was located at the origin of a lattice of unit spacing. Another particle was launched far from the origin and was allowed to walk at

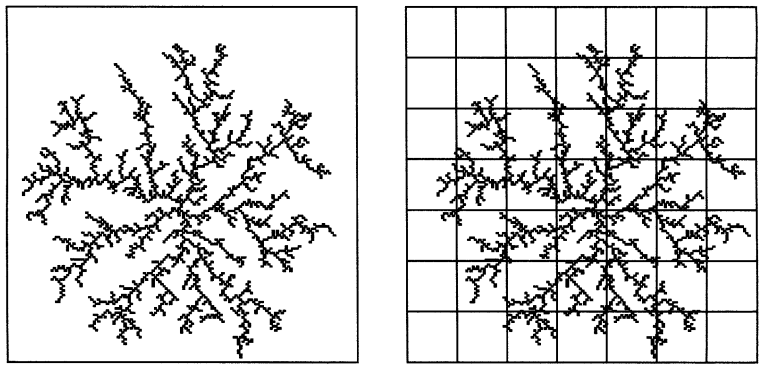

Fig. 1 (a) Typical cluster obtained for five "active sites" for each particle. (b) B–C method: the cluster has been put into a regular lattice of "s" amplitude. In this case, $s = 1/7$

random (diffuse) until it arrived at a site adjacent to the seed particle and remained fixed to it. Another particle was launched which stopped when adjacent to the occupied sites, and so forth. In this way large clusters could be generated whose structure was expected to be characteristic for objects grown under diffusion-limited conditions [2].

If a particle in its random walk touched the lattice boundary, it was discarded and another one was introduced [4]. The simulation went on until the desired number of particles for the cluster was completed. The largest number considered was 2000 particles for each cluster. The program was adapted to introduce a variable number (from 3 to 8) of interaction "active sites" for each particle for its addition to the aggregate. First, the four sides and the four vertexes of each particle were considered as equivalent active sites (eight sites) with the same probability to be occupied. Then, seven sites were randomly chosen, from the eight available ones. And so forth until the number of randomly chosen sites reached a value of 3.

To study the effect of definite configuration of active sites for a given number of sites, from all the possible configuration a few ones were selected and maintained fixed during all the aggregation process.

Besides the program enabled us to count the particles having different number of occupied sites and calculate the average number of occupied sites by particle.

Determination of the fractal dimension

The structure of the aggregates was characterized by the so-called box-counting (B–C) method. The aggregate was put into a regular lattice of "s" amplitude. The number of squares having something of the structure was counted giving a number N: $N = N(s)$. Diminishing "s" the corresponding $N(s)$ were obtained. A doubly logarithmic plot of $N(s)$ versus $1/s$ was a straight line with a slope equal to the fractal dimension of the aggregate (Fig. 1).

Fig. 2 Fractal dimension as a function of the number of active sites for each particle

Results and discussion

At least 10 runnings of the program were made to obtain different clusters for each number of active site as described before. The results obtained for random or fixed configurations were very similar (Fig. 2). Both kinds of configurations presents nearly the same fractal dimension confirming the results obtained by other authors [5]. For increasing number of aggregated particles until 2000, the fractal dimension tended to 1.70 as was reported for 2d aggregation by several authors. The results of Figs. 3 and 4 showed that the average number of occupied sites by particle tended to reach a maximal value which was almost the same in spite of either the number of available sites on the particle, or the configuration of these sites.

It appears that the knowledge of the fractal dimensionality of the cluster is not sufficient to characterizing the interaction surface of particles when they come into contact to form larger aggregates.

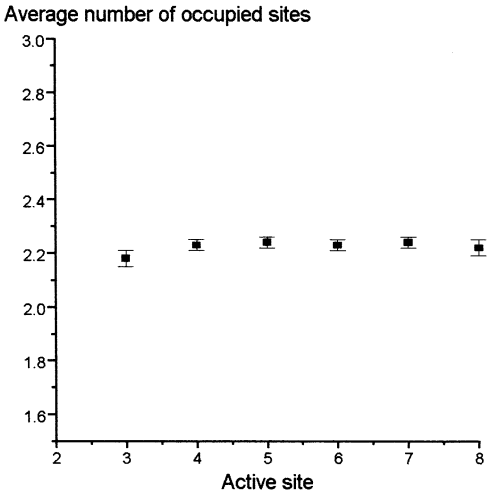

Fig. 3 Average number of occupied sites per particle as a function of the number of available sites on the particle

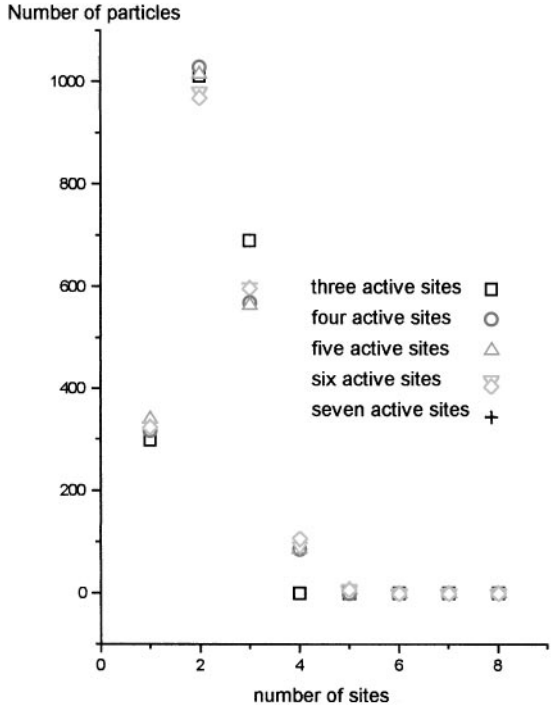

Fig. 4 Number of particles as a function of the number of occupied sites. Most of the particles have two sites occupied no matter which the number of available sites on the particle is

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