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Influence of particle size on diffusion-limited aggregation

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The influence of particle size on diffusion-limited aggregation (DLA) has been investigated by computer simulations. For DLA clusters consisting of two kinds of particles with different sizes, when large particles are in the minority, the patterns of clusters appear asymmetrical and nonuniform, and their fractal dimensions D_f increase compared with one-component DLA. With increasing size of large particles, D_f increases. This increase can be attributed to two reasons: one is that large particles become new growth centers; the other is the big masses of large particles. As the concentration ratio x_n of large particles increases, D_f will reach a maximum value D_{f_m} and then decrease. When x_n exceeds a certain value, the morphology and D_f of the two-component DLA clusters are similar to those of one-component DLA clusters. [S1063-651X(99)05510-5]

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I. INTRODUCTION

Recently, there has been increasing interest in a variety of nonequilibrium aggregation models such as diffusion-limited aggregation (DLA), introduced by Witten and Sander [1–7]. A large number of computer simulations, theoretic analyses, and experiments have been carried out to investigate the relationship between the cluster geometry and growth mechanisms. The DLA model is a simple idealization of a common natural process, the formation of natural objects where the rate-limiting step is diffusion. In two dimensions, its fractal dimension D_f is about 1.71 and there exists no exact formula for the fractal dimension [7–12]. The DLA presents a prototype of the pattern formation of diffusive systems including the electrochemical deposition, crystal growth, viscous fingering, dielectric breakdown, and colloid aggregation [13–21].

Although the effect of particle size for the DLA cluster is significant [10], not much attention has been given to the subject and most of the existing theoretical models do not predict the particle size effect on morphology and fractal dimension of DLA. Ossadnik, Lam, and Sander have simulated a variant of DLA in which the sizes of particles are given according to a power-law distribution. In that case, they obtained the relation of fractal dimension to distribution exponent [10]. But there is still a lack of understanding of the relation between particle size and characteristics for DLA clusters.

In this paper, we investigate the general relations of particle size to morphology and the fractal dimension of two-component DLA clusters by Monte Carlo simulations. These results will be useful for the further understanding of DLA model.

II. SIMULATIONS

We consider the two-component DLA cluster. The diameter of small particles is taken as length unit. The reduced diameter of large particles is σ_m. The concentration ratio of large particles is x_n. The algorithms in our off-lattice two-component DLA simulations are almost similar to those in Refs. [6,7], except for the flight distance of a random walker $d=d_{\min}-\rho l$, where $d_{\min}$ is the distance from the random walker to the closest aggregated particle. l is the sum of radii of the two particles and ρ stands for a certain factor. In this simulation, ρ is taken as 0.95, which means that the parts of the aggregated particles do not overlap much and algorithms can be carried out at relatively high speed.

The cluster can be generated as follows: Random particles are launched at a random position on a circle of radius $R_{\max}+\delta+\sigma^*/2$ centered on the immobile seed, where $R_{\max}$ is the outer radius of the cluster, δ is chosen to be three times the reduced diameter of small particles as used generally [6,7], and σ^* represents reduced diameter of the walker. At every step, $d_{\min}$ is determined. If $d_{\min}<l$, the particle stops diffusion and becomes a part of the cluster. Otherwise, it jumps to a random position on a circle of radius $(d_{\min}-\rho l)$ centered on the walker. If the distance from a walker to the seed is too large ($>4R_{\max}$, here), it is killed and a new random particle is released. In this way, starting from an immobile seed, the cluster grows when a walker hits it and becomes a part of it. During growth of DLA clusters, a particle with reduced diameter σ^* is produced randomly according to

$$\sigma^*=\begin{cases}\sigma_m^*, & p<x_n\\ 1, & p\geqslant x_n\end{cases} \tag{1}$$

where p stands for a random number between 0 and 1. For the two-component DLA clusters, the scaling form [2,3,10]

$$M\sim R_g^{D_f} \tag{2}$$

can be used to calculate the fractal dimension, where D_f is the fractal dimension. M and R_g stand for the mass and radius of gyration of the cluster, respectively. They can be determined as follows: Let σ_i^* and $\mathbf{r}_i$ represent the reduced diameter and position of the ith particle in a cluster. Assuming every particle is uniform, the mass of the ith particle is $m_i=\pi(\sigma^*)_i^2/4$. Then the mass and radius of gyration of the cluster are given by [2,10]

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$$M = \sum_{i=1}^{N} m_i, \tag{3}$$

$$MR_g^2 = \sum_{i=1}^{N} m_i[(\mathbf{r}_i - \mathbf{r}_c)^2 + \sigma_i^2/8], \tag{4}$$

where $\mathbf{r}_c$ is the position vector of the mass center of the cluster and N is the particle number of the cluster.

III. RESULTS AND DISCUSSION

We investigate the morphology and fractal dimension for DLA clusters consisting of two kinds of particles with different sizes.

The number of particles is $N=10\,000$ in these simulations. Reduced diameters of large particles are taken as $\sigma_m^*=10$, 20, 30, 40, and 100, and the concentration ratios x_n of large particles are chosen to be 0.001, 0.002, 0.005, 0.01, 0.02, 0.05, and 1, respectively.

Figure 1 gives the morphologies of the one-component DLA cluster (a); two-component DLA cluster with $x_n=0.001$ and $\sigma_m^*=20$ (b); and two-component DLA cluster with $x_n=0.02$ and $\sigma_m^*=20$ (c). It can be seen that the one-component DLA cluster is relative symmetrical and uniform [see Fig. 1(a)]. But, when a few large particles are mixed in the cluster, the pattern of cluster appears asymmetrical and large particles become new growth centers around which other particles grow and form new branches [shown in Fig. 1(b)]. It is also found that, when the size of large particles increases, the asymmetry and nonuniformity of DLA clusters appear more apparent, and branches around large particles become denser. As the concentration ratio x_n of large particles rises, the pattern of cluster changes from asymmetry to symmetry gradually. And after x_n reaches a certain value, its morphology is similar to that of the one-component DLA cluster [see Fig. 1(c)].

Fractal dimensions are calculated for DLA clusters composed of two kinds of particles with different sizes by using Eq. (2). The statistic mean must be carried out because of the asymmetry and nonuniformity of the two-component DLA clusters. The numbers of clusters used for the statistic mean are 60, 40, and 20 for the systems with $\sigma_m^*=30$, 20, and 10, respectively. Figure 2(a) gives the fractal dimension D_f versus the concentration ratio x_n. It can be seen, when a few large particles are put into the DLA cluster, that D_f will increase comparing with that of the one-component DLA cluster. It can also be found, with the size of large particles rising, that the fractal dimension increases from 1.71 to 2. As x_n continues to rise, D_f will reach a maximum value D_{f_m}, and then decrease. When x_n exceeds a certain value, D_f will stay constant and be equal to that of one-component DLA, i.e., about 1.71. Our simulations also show that there is no effect on morphology and fractal dimension when a few small particles are added into DLA clusters. It is not surprising that only a few large particles make the fractal dimension of the two-component DLA cluster change from 1.71 to 2. Figure 2(b) shows the fractal dimension versus the mass ratio x_m of large particles. It can be seen that when the fractal dimension reaches the maximum, the mass ratio of large particles reaches a large value too. For example, the maximum fractal dimension corresponds to x_m of 70. Figure 3 plots maximum fractal dimension D_{f_m} as a function of reduced diameter σ_m^* of large particles. D_{f_m} increases with rising σ_m^*. When $\sigma_m^*\geqslant 40$, D_{f_m} approximates to 2, the value of the spatial dimension.

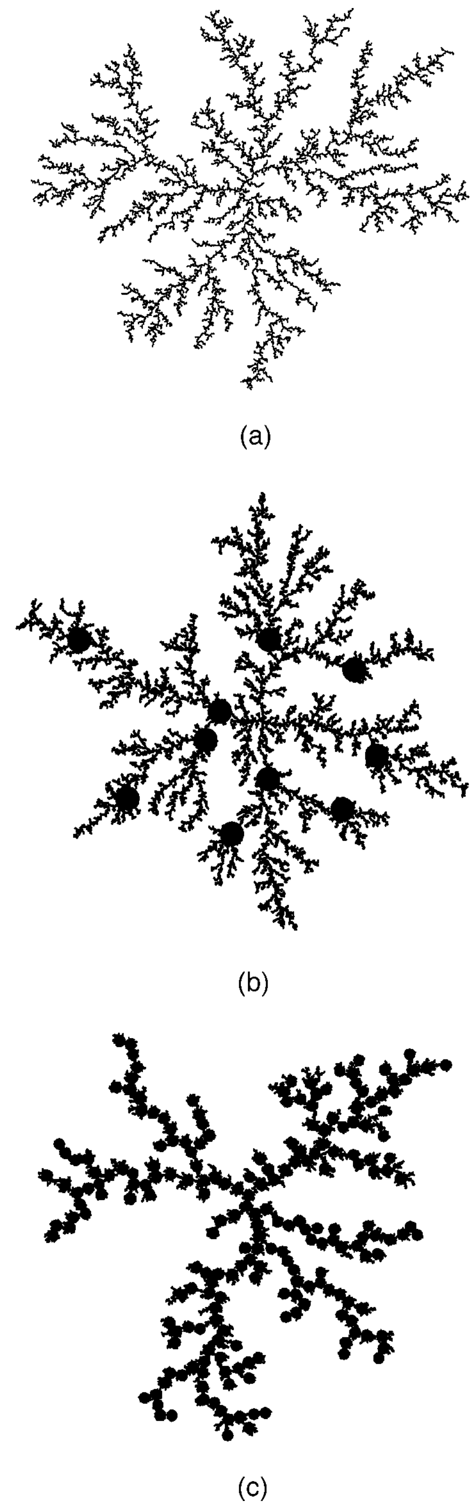

FIG. 1. Morphologies of clusters: (a) one-component DLA cluster; (b) two-component DLA cluster for $x_n=0.001$, $\sigma_m^*=20$; (c) two-component DLA cluster for $x_n=0.02$, $\sigma_m^*=20$.

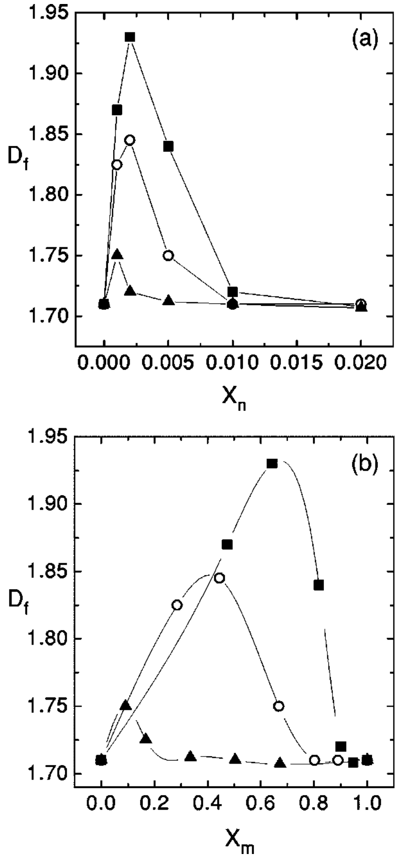

FIG. 2. Fractal dimension of two-component DLA clusters versus concentration ratio x_n of large particles (a) and mass ratio x_m of large particles (b). Reduced diameter of large particles: $\sigma_m^*=30$ (solid square), 20 (open circle), and 10 (solid triangle).

It can be seen from Fig. 1(b) that the increase of fractal dimension of the two-component DLA cluster comes from two parts: forming new growth centers and increasing mass due to substitution of large particles for small ones. To study effects of the new growth centers on increase of fractal dimension, we consider the pseudo-one-component DLA cluster in which the arrangement of particles is the same as the corresponding two-component DLA clusters, but large particles are replaced by small ones. This kind of clusters have two significant characteristics: one is that there are the same morphologies (especially, dense branch structure) as that of corresponding two-component DLA clusters; the other is that there is no large particle, i.e., there is no effect of the big masses of large particles. Fractal dimensions D_f^p of the pseudo-one-component clusters are calculated and shown in Fig. 4(a). They are larger than those of the one-component DLA cluster but smaller than those of the two-component DLA clusters. The increase δD_f of fractal dimensions can be divided into two parts: $\delta D_f=\delta D_f^1+\delta D_f^2$. δD_f^1 is due to the contribution of new growth centers and presented by $\delta D_f^1=D_f^p-1.71$, where 1.71 is the fractal dimension of the one-component DLA clusters; δD_f^2 results from big masses of large particles and is written as $\delta D_f^2=D_f-D_f^p$, where D_f represents fractal dimensions of corresponding two-component DLA clusters. Figures 4(a) and 4(b) show δD_f^1 and δD_f^2 as functions of concentration ratio x_n of large particles, respectively. It can be seen from these figures that $\delta D_f^1<\delta D_f^2$. Thus, we come to the conclusion that the big mass of large particles plays an important part in the increase of fractal dimension for two-component DLA clusters when x_n is small.

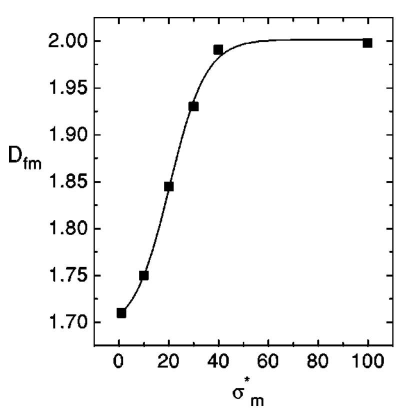

FIG. 3. Maximum fractal dimension D_{f_m} of two-component DLA clusters as a function of reduced diameter of large particles.

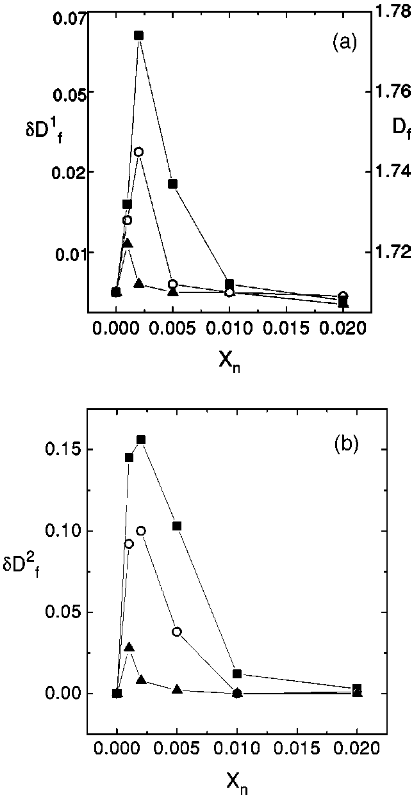

FIG. 4. (a) Increasing part δD_f^1 of fractal dimension for the dense branch structure versus concentration ratio of large particles (right Y axis represents fractal dimensions D_f^p of pseudo-one-component DLA clusters); (b) increasing part δD_f^2 of fractal dimension resulting from big masses of large particles versus concentration ratio of large particles. Reduced diameter of large particles: $\sigma_m^*=30$ (solid square), 20 (open circle), and 10 (solid triangle).

IV. CONCLUSION

We have studied two-component DLA clusters consisting of two kinds of particles with different sizes by off-lattice simulations. With the number of large particles rising, the morphology of two-component DLA clusters changes from relative symmetry and uniformity to asymmetry and nonuniformity, then returns to relative symmetry. Corresponding to the change of morphology, the fractal dimension of the two-component DLA clusters increases from 1.71, the fractal dimension of the one-component DLA cluster, to the maximum, then decreases to about 1.71.

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