Particle-cluster aggregation on a small-world network

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To describe the aggregation behaviors on substrates with long-range jump paths, a model of particle-cluster aggregation on a two-dimensional small-world network is presented. This model is characterized by two parameters: the clustering exponent α and the long-range connection rate ϕ. The results show that there exists an asymptotic fractal dimension $D_f^{\max}$ that depends upon α. With decrement of α, $D_f^{\max}$ varies from 1.7 to 2.0, which corresponds to a crossover from diffusion-limited-aggregation-like to dense growth. The change of the aggregation pattern results from the long-range connection in the network, which reduces the effect of screening during the aggregation. When the system size is not large enough, the effective fractal dimension D_f depends upon ϕ because of the finite-size effect. With primitive analysis, we obtain the expression of the effective fractal dimension D_f with the network parameters α and ϕ.

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During the past two decades, the far-from equilibrium growth phenomena have been extensively investigated both experimentally and theoretically because of their relevant applications in many fields of science and technology [1–6]. The structure of growing patterns strongly depends on the dynamics of the growth process. Many efforts have been directed to the development of growth models in order to account for the existing fractal patterns [7–14]. The diffusion-limited aggregation (DLA), which was introduced by Witten and Sander, is probably the most widely known growth model [8]. The DLA and its variants can recur in many fractal patterns in diffusive systems, including electrodeposition, colloid aggregation, crystal growth, viscous fingering, dielectric breakdown, etc. [1–3].

In the DLA model, the particle jumps from the current site to one of their *nearest neighbors* at each step, performing purely random walks, until it hits and sticks to the cluster [8]. However, in some physical processes, except nearest-neighboring jumps, there also exist some long-range jumps through which the particle can move to a distant site at a step. An example is the Lévy flight of particles in the processes such as bulk-mediated surface diffusion, transport in micelle systems, and heterogeneous rocks [15], in which the jump distance follows a power-law distribution. Another example is the diffusion of adatoms on metal surfaces, which is important for the thin-film growth, heterogeneous catalysis, and oxidation [15]. In this case, a bunch of defects or impurities in the substrate may play the part of the long-range jump path. In the cases of weak adsorbate-substrate interaction, the long jumps, spanning multiple lattice spacings, also play a dominating role for the surface diffusion [16]. In this Brief Report, we introduce the notion of a small-world network [17] into the investigation of the aggregation of particles with long-range diffusion. The basis idea is that, regarding the lattice point of the real space as the node of the network, the jumps of particles in real space correspond to the links in the network.

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The small-world network [17–26] is suitable to describe the distribution of the short- and long-range paths for the diffusion of particles in the substrate. Usually, there are two methods to build a small-world network. One is by randomly rewiring the original links of the regular lattice, and the other is by adding the random links to the regular lattice. The networks created by using these two methods have very similar scaling characters [17–19]. However, for the network created by rewiring the original links, there probably exist isolated sites which have no link to any other sites of the system; but for the network created by adding the random links, there is no isolated site. Thus, considering the continuity of the real space, we use the addition of the random links to build the small-world network. We build the network on the basis of a square lattice of size $L_{\mathrm{nw}} \times L_{\mathrm{nw}}$ with periodic boundary conditions. Each site in the lattice is connected to its four nearest-neighboring neighbors, representing nearest jumps. Then, a long-range connection, denoting a long-range jump, is added between two randomly chosen sites with the probability [15,22–24]

$$p(r) \sim r^{-\alpha}, \tag{1}$$

where r is the Euclidean distance between two selected sites and α ($\alpha \geqslant 0$) is a model parameter. This process is repeated until the ratio ϕ between the number of long-range connections and that of short-range ones reaches a desired value. Thus, the average coordination number per site is $4(1+\phi)$ in the present small-world network. When the parameter $\alpha=0$, we have a uniform distribution over long-range connections, and the present model reduces to the basic small-world network [25]. As α increases, the long-range connections of a site become more and more clustered in its vicinity. Thus, α serves as a structural parameter measuring how widely "networked" the underlying society of sites is. The parameter α is called the clustering exponent, which characterizes the localized degree of the long-range connections in the network.

Based on the small-world network as created above, we describe how the particles aggregate. First, a particle is launched at a random position on a circle of radius

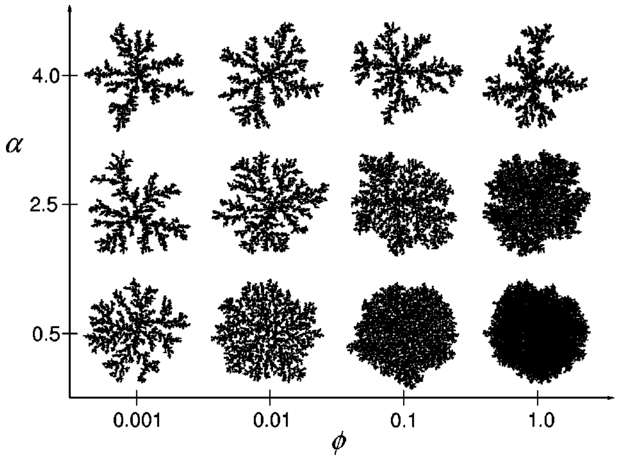

FIG. 1. Patterns of the clusters as a function of the long-range connection rate ϕ for several clustering exponents α.

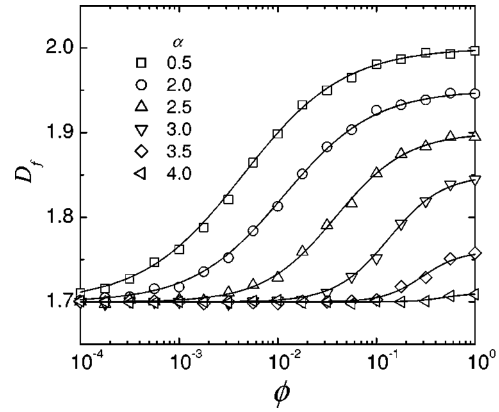

FIG. 2. The effective fractal dimensions D_f of the clusters as a function of the long-range connection rate ϕ for a set of α. The symbols are the simulation results, and the lines are the plots of Eq. (3).

$R_s(=R_{\max}+\Delta R)$ centered on the original cluster, where $R_{\max}$ is the outer radius of the cluster and ΔR is chosen so that $\Delta R^{-\alpha}\approx 10^{-4}$ if possible. The motivation for the choice of R_s is to ensure that there is only a small probability that the particle will contact the cluster during the first step in the movement. Then the particle jumps from the current site to one of its linked sites which are not occupied by the growing cluster, with equal probability step by step. It ensures that any site in the cluster has only one particle. This moving rule is reasonable because we focus on the two-dimensional pattern of the cluster. The particle stops and sticks to the cluster permanently when it moves into a site which is the nearest neighbor of the growing cluster in terms of the Euclidean distance. In this way, starting from an immobile seed, the cluster will grow gradually when a particle hits it and becomes a part of it.

We have performed extensive numerical simulations for the particle-cluster aggregation on the small-world network with size $L_{\mathrm{nw}}=2000$. To reduce the effect of fluctuation, for each set of parameters (α,ϕ) the calculated result is taken from the averaging over ten different network realizations and at least 10 independent runs for each network realization.

Figure 1 shows the simulation patterns of aggregates as a function of the long-range connection rate ϕ for several clustering exponents α for clusters with number of particles $N=10\,000$. It can be seen that as the parameters α and ϕ vary, the patterns of aggregates exhibit rich behaviors. For small α, with the increase of ϕ the patterns of aggregates evolve from the thin and sparse branching structure to the thick and dense branching one, and finally to a compact cluster one. However, for large α the patterns of aggregates almost do not vary with ϕ, and remain a kind of prototype disorder structure. To quantify the patterns of aggregates, we calculate the fractal dimensions D_f of the aggregates, which are shown by symbols in Fig. 2.

It can be seen from Fig. 2 that the fractal dimension D_f tends to an asymptotic value $D_f^{\max}$ as the long-range connection rate ϕ is large enough. As expected, the asymptotic fractal dimension $D_f^{\max}$ depends on the clustering exponent α. However, it is hard to understand how the fractal dimension D_f shows a strong dependence on the long-range connection rate ϕ. This is due to the finite system size. It is plausible to imagine that there exists a special length L for given values α and ϕ. When the length of the cluster $R_{\mathrm{cluster}}\gg L$, the long-range connection strongly affects the morphology of the aggregate, and the fractal dimension D_f takes the asymptotic value $D_f^{\max}$. When $R_{\mathrm{cluster}}\ll L$, the effect of the long-range connection is restrained and the aggregate maintains the DLA cluster. For intermediate size of the cluster, R_{cluster} is comparable to L, and D_f takes an intermediate value. The special length L depends on the clustering exponent α and long-range connection rate ϕ. ϕ determines the amount of long-range connections, so L increases as ϕ decrease. α indicates the distance restriction of the long-range connection, therefore L decrease as α reduces. In the present simulation, the particle number of the cluster $N=10\,000$. When $\phi=10^{-4}$, about one long-range connection exists in the area of the cluster. As expected, $R_{\mathrm{cluster}}\ll L$ and $D_f\approx 1.7$ for all α (see the left side of Fig. 2). On the contrary, when ϕ is large and α is small (e.g., $\phi=1$ and $\alpha=0.5$ or 2), L is so small that the condition of $R_{\mathrm{cluster}}\gg L$ is met. In this case, D_f reaches its asymptotic value $D_f^{\max}$ (see the right side of Fig. 2). In the intermediate region, L varies from a large value to a small one relative to the size of the cluster, and D_f changes from the fractal dimension of pure DLA to the asymptotic one, correspondingly. The value of D_f depends on the size of the cluster, so we might regard it as the effective fractal dimension. The true asymptotic scaling is obtained only from $R_{\mathrm{cluster}}\gg L$, making D_f independent of ϕ.

Now we turn to deduce a rough expression of the effective fractal dimension D_f as a function of ϕ for various α. The growth of the cluster comes from two contributions: one is the nearest-neighbor links in the underlying regular lattice, and the other is the effective long-range links. We take the effect of the underlying regular lattice on the effective fractal dimension D_f as unit 1, and assume that the contribution of effective long-range connections to D_f is proportional to ϕ with the power θ as

$$\Gamma = B(\alpha)\phi^{\theta(\alpha)}, \tag{2}$$

where B is a proportional factor. The exponent θ expresses the effectiveness of the long-range connection and it depends

TABLE I. The parameters $D_f^{\max}$, B, and θ in Eq. (3) for various α values.

α	0.5	2.0	2.5	3.0	3.5	4.0
$D_f^{\max}$	2.0	1.95	1.9	1.85	1.76	1.71
B	100	70	50	25	15	10
θ	0.85	0.95	1.2	1.6	2.2	3.0

on α. Thus, we obtain the effective fractal dimension D_f as the form

$$D_f(\alpha,\phi) = D_f^{\mathrm{DLA}} + \frac{B\phi^{\theta}}{1+B\phi^{\theta}}(D_f^{\max} - D_f^{\mathrm{DLA}}), \tag{3}$$

where D_f^{DLA} is the fractal dimension of the pure DLA with a value of about 1.7, and $D_f^{\max}$ is the asymptotic value of the fractal dimension of the cluster for large ϕ which can be obtained from the simulation data. The first term on the right side of Eq. (3) corresponds to the contribution of the underlying regular lattice. The second term takes into account the increase of the fractal dimension resulting from the effective long-range connections. Fitting the simulation results shown in Fig. 2 by using Eq. (3), the fitting parameters B and θ are obtained and listed in Table I.

We also investigate the influence of the clustering exponent α on the aggregating behavior of particles. Figure 3 shows the effective fractal dimension D_f as a function of α for three typical long-range connection rates ϕ. For large α (e.g., $\alpha > 4$ in Fig. 3), the long-range connection is short-ranged essentially, and the aggregate appears to be a DLA cluster. In this case, $D_f \approx 1.7$ for all ϕ. As α decreases, the length of the long-range connection becomes larger, and the long-range connections make a contribution to the morphology of the aggregate more and more. Correspondingly, D_f increases from 1.7 to 2.0. In Fig. 3, the D_f-α relation depends upon ϕ. It comes from the effect of the finite system

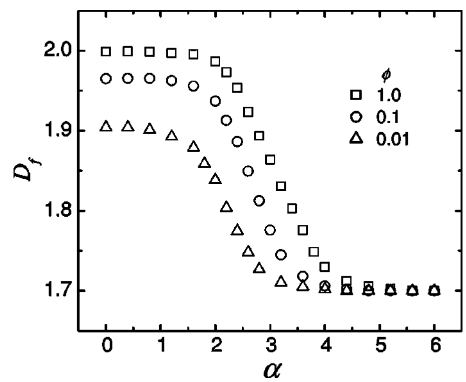

FIG. 3. The effective fractal dimensions D_f of the clusters as a function of the clustering exponent α for several fixed ϕ values.

size. It can be seen from Fig. 3 that when α is small enough ($\alpha < 1$), D_f does not vary with ϕ any longer and it reaches the asymptotic value $D_f^{\max}$ for the present system with a particle number of $N = 10\,000$. In the other case, the finite system size has an effect on the morphology of the aggregate and D_f varies with ϕ.

In summary, we investigate the particle-cluster aggregation on the substrates with both short-range jump paths and long-range ones. The substrate is expressed as a small-world network with the parameter α and ϕ. Thus, the behavior of the aggregation pattern can be characterized by the parameters of the small-world network. As the clustering exponent α and long-range connection rate ϕ vary, the pattern of the aggregate crosses over from the DLA-like pattern to the dense growth one, and the fractal dimension changes continuously from about 1.7 to 2.

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