Two-dimensional magnetic cluster growth with a power–law interaction

Xiaojun Xu a,*, Yiqi Wu b,c, Gaoxiang Ye c

a Department of Applied Physics, Zhejiang University of Technology, Hangzhou 310032, PR China
b Wenzhou University Oujiang College, Wenzhou 325027, PR China
c Department of Physics, Zhejiang University, Hangzhou 310027, PR China

Received 26 September 2007; received in revised form 31 October 2007; accepted 1 November 2007
Available online 21 December 2007

Abstract

A two-dimensional cluster model in which the morphology of clusters depends on power–law magnetic interactions that decay with distance \( r \) as \( r^{-\alpha} \) is introduced. The growth algorithm is a generalization of diffusion-limited aggregation (DLA) model. The particles with spin degree diffuse on a square lattice and each spin is allowed to flip under a Monte Carlo probability. The simulation shows that, for the antiferromagnetic coupling, the spins of the particles in clusters tend to be oriented alternately. For the ferromagnetic coupling, however, the spin distribution depends on the exponent \( \alpha \): for large value of \( \alpha \), domains with different sizes are observed in the clusters; while for small \( \alpha \), during the earlier stage of the growth process, the clusters exhibit approximately antiferromagnetic structure, then, in subsequent growth of the outer part of the clusters, the spin states of all particles are similar. The magnetization and system energy of the clusters as well as their evolutions with the growth parameters are also studied in detail.

© 2007 Elsevier B.V. All rights reserved.
PACS : 61.43.Hv; 05.50.+q; 64.60.Ak; 82.20.wt

Keywords: Diffusion-limited aggregation; Power–law interactions; Spin distribution; Magnetization; Energy

1. Introduction

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 [1–5]. 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 [6–10]. Among the models, diffusion-limited aggregation (DLA) model is very applicable, which was introduced in 1981 by Witten and Sander [6]. The DLA model and its variants provide a basis for understanding a large number of natural formation phenomena, including electrodeposition, colloid aggregation, crystal growth, viscous fingering, dielectric breakdown, etc. [1–3]. However, many of the questions concerning structure formation and transitions between different growth morphologies have not so far been satisfactorily answered. Much effort has especially been devoted to establishing the relationship between cluster morphology and the growth mechanism.

In the DLA model, the diffusing particle jumps from the current site to one of its nearest neighbors at each step, performing purely random walks without any interactions among particles, until it hits and sticks to the cluster [6]. However, in many physical processes, there also exist especially some long-range interactions [11–17], which are important in determining the aggregation of particles. Typical examples are gravitational and Coulomb interactions, where the potential decays with distance \( r \) as \( 1/r \). Several other important examples can be found in condensed matter, such as dipolar (both electric and magnetic) and Ruderman–Kittel–Kasuya–Yosida (RKKY) interactions, both proportional to \( 1/r^3 \). Effective interactions with a power–law decay \( 1/r^\alpha \), with some exponent \( \alpha \geq 0 \), appear also in other related problems such as critical phenomena in highly ionic systems [18], Casimir forces between inert uncharged particles immersed in a fluid near the critical point [19], and phase segregation in model alloys [20].
In this paper we study, by Monte Carlo simulation, the growth of clusters in the DLA model with spin degree exhibiting power–law coupling interactions. Our purpose is to analyze comprehensively the influence that these interactions have in the kinetics of aggregation in a simple numerical model, such as the spin distribution, magnetization and system energy of the clusters.

2. Computational model

The model used in this work is based on the DLA model with the addition of a spin freedom (up or down) in each particle. The probabilities of jumping to one of the four neighbor sites and spin orientation are defined as proportional to \( \exp(-\Delta H) \), where \( \Delta H \) is the local gain of the dimensionless coupling energy between the initial and the final states defined by

\[
H = -\frac{\beta}{2} \sum_{ij} J(r_{ij}) S_i S_j \quad (S_i = \pm 1 \forall i),
\]

(1)

with

\[
J(r_{ij}) = \frac{C}{r_{ij}^a} \quad (a \geq 0),
\]

(2)

(where \( r_{ij} \) is the distance in lattice units) between particle \( i \) and \( j \), and the sum \( \sum_{(i,j)} \) in Eq. (1) runs over all distinct pairs of particles. \( C \) is considered to be an exchange integral, while \( \beta \) is a parameter such that \( \beta C \) is dimensionless, and \( a \) corresponds to the distance dependence of coupling interactions. For large value of \( a \), the interaction between two particles decays rapidly with distance, therefore, the system exhibits short-range interaction behavior. While for small \( a \), the interactions are almost distance independent, i.e., long-range interaction system.

For more detailed description of the model, our previous paper [21] is suggested.

3. Results and discussion

Fig. 1 gives a typical cluster containing the first 500 particles grown from an up spin as seed with \( \beta C = -5 \) and \( a = 2 \). White and black dots represent up and down spins, respectively. It can be seen from Fig. 1 that, for negative value of \( \beta C \), an antiferromagnetic ordering is favored during the growth, i.e., an incoming spin tends to be oriented conversely to the orientation of its nearest neighbors in the cluster. The two components are, therefore, equally distributed in the cluster. It should be noted that this distribution of spins in Fig. 1 is almost same with negative value of \( \beta C \) for different \( a \).

On the contrary, for positive value of \( \beta C \), the effects of magnetic power–law interactions on the spin distributions of the clusters become important.

For larger value of \( a \) which exhibits short-range magnetic interactions, some domains or segments are found in branches in the same spin state, which is either up or down (ferromagnetic ordering). With \( \beta C < 0.3 \) for the case of \( a = 5 \), the spins in the cluster are oriented randomly during the magnetic DLA growth. If \( \beta C \) ranges from 0.5 to 3, as shown in

Fig. 1. Spin distribution of the cluster containing the first 500 particles grown with \( a = 2 \) and \( \beta C = -5 \). White and black dots represent up and down spins, respectively.

Fig. 2(a and b) for the clusters containing the first 500 particles, the clusters become ferromagnetic ones, and the scale of domains increases with \( \beta C \). When \( \beta C \) ranges from 5 to 8, domain structure disappears and the spins of all particles in each branch are found to be identical, as seen from Fig. 2(c). As \( \beta C \) further increases, the whole cluster is in one spin state—the state of the seed.

When the diffusing particle is far away from the cluster, due to the short-range interactions, the value of \( 1/r^a \) in Eq. (2) is almost independent on the distance \( r \). Therefore, the motion of the diffusing particle is Brownian when it moves toward the cluster and the spin flips randomly. However, if the diffusing particle moves near to the cluster, in particular, it reaches a neighboring site of the perimeter, the diffusion is controlled by the local “magnetic” configuration on the surface of the cluster. The probability to keep the diffusing particle and it’s connected one in the cluster in a same spin state (i.e., ferromagnetic ordering) is larger than the probability of spin-flip. It is easy to figure out that, in terms of the statistical principle, the scale of domain in the cluster depends on the ratio of the above two probabilities, which is determined by the value of \( \beta C \). By varying \( \beta C \) to change the ratio of two probabilities, a different scale of domain is found, as seen in Fig. 2(a–c). As \( \beta C \) further increases, the probability of overturn tends to zero and the whole cluster is in one spin state.

Fig. 2(d) gives a typical cluster containing the first 500 particles grown with \( a = 2 \), \( \beta C = 1 \). It can be seen that, for \( a = 2 \), there also have domains in cluster, like the case of \( a = 5 \). However, as shown in Fig. 2(d), the scales of the domains are quite different. There have many “monoparticle domains”, which means that the orientation of the spin next coming will overturn frequently. Along with the value of \( \beta C \) being larger, the probability of overturn becomes smaller, therefore, the number of “monoparticle domain” decreases. As \( \beta C \) further increases, the whole cluster will be in one spin state—the state of the seed.

For \( a = 2 \), the growth process exhibits medium–range magnetic interactions, the aggregation of particles moving
towards the cluster is through a Brownian motion and the spin is oriented randomly, when the diffusing particles are far away from the cluster, as the case of short-range interactions. However, if the particle is near to the cluster, the power–law interactions become stronger which are not only affected by the nearest neighbor particles but also influenced by all particles around it. Therefore, it possesses the properties of the case of short-range interactions, i.e., domains in branches, but differs from it: the scales of the domains are quite different and “monoparticle domain” appears.

In order to further understand the competition of two spin states on the kinetic growth process, we measured the dependence of the maximum domain size \( S_{\text{max}} \) and the average domain size \( \langle S \rangle \) in each cluster of 2000 particles on the coupling \( \beta C \) for the cases of \( \alpha = 2 \) and 5, and the results are shown in Fig. 3. It is found from Fig. 3(a) that, the maximum domain size \( S_{\text{max}} \) increases from 16 to 2000 in a 2000 particles cluster with \( \beta C \) increases, and a sharp variation appears in the case of \( \alpha = 2 \) compared to that of \( \alpha = 5 \). Again we observe, a similar behavior of the evolution of average domain size \( \langle S \rangle \) in each cluster of 2000 particles with the coupling parameter \( \beta C \) is shown in Fig. 3(b) with \( \langle S \rangle \) increases from 1.5 to 2000.

For small value of \( \alpha \), as seen in Fig. 4 with \( \alpha = 0.5 \), the core regions of the clusters, which are aggregated at earlier stage of the growth, are nearly in antiferromagnetic state and the outside of the core regions are in the same spin state (which is either up or down). When \( \beta C \leq 0.01 \), the spins in clusters are oriented randomly. If \( \beta C \) ranges from 0.03 to 0.5, the size of the core regions with likely antiferromagnetic spin distribution decreases for the case of \( \alpha = 0.5 \), as shown in Fig. 4, and only about 10

Fig. 2. Spin distribution of four clusters containing the first 500 particles with different values of \( \beta C \) and \( \alpha \). (a) \( \alpha = 5, \beta C = 0.5 \); (b) \( \alpha = 5, \beta C = 2 \); (c) \( \alpha = 5, \beta C = 5 \) and (d) \( \alpha = 2, \beta C = 1 \).

Fig. 3. Evolution of the maximum domain size \( S_{\text{max}} \) (a) and the average domain size \( \langle S \rangle \) (b) in each cluster of 2000 particles with the coupling parameter \( \beta C \), with \( \alpha = 2 \) (solid triangle) and \( \alpha = 5 \) (open square), respectively. The solid line between the data points is the guide to the eye.
particles are in antiferromagnetic state as $\beta C = 0.5$. While $\beta C$ larger than 0.8, the whole particles in one cluster are in a same spin state.

The evolution of spin distribution in the magnetic DLA growth with long-range interactions is also studied, and the simulation results for the number of up spins aggregated to the cluster as a function of the $N$th 100 particles during the growth process for a set of $\beta C$ are shown in Fig. 5 with (a) $\alpha = 0.5$ and (b) $\alpha = 0.1$, respectively. The point A(10,83) in Fig. 5(a) means that, for the cluster growth with $\alpha = 0.5$ and $\beta C = 0.03$, there are 83 up spins in the next coming 100 particles aggregate to the cluster with 900 particles existed earlier. It can be seen that, when $\beta C = 0.01$, the number of up spins is about 50 during the whole growth process, which means the up and down spins are equally distributed in the cluster. However, as shown in Fig. 5(a) for $\beta C = 0.03$, the number of up spins changes gradually from 50 to 100 when $N$ increases from 7 to 16. This behavior can be explained intuitively from Fig. 4. During the earlier stage of growth process, the two spin states are equally distributed in approximately antiferromagnetic structure firstly. Then, one of them becomes dominant in quantity. At last, in subsequent growth of the outer part of the cluster, the spin states of all particles are similar, as shown in Fig. 4. The critical value of $N$, where the number of up spins presents a marked variation from about 50, decreases with $\beta C$. Furthermore, a similar behavior of the evolution of spin distribution for the case of $\alpha = 0.1$ is shown in Fig. 5(b).

In order to numerically investigate the competition between two spin species, the magnetization $M$ of the magnetic DLA clusters have been measured, which is defined as the difference between the number of up and down spins in the cluster, normalized by the mass $N$ of the cluster. Fig. 6 shows the magnetization $M$ of the cluster containing 2000 particles as a function of the coupling $\beta C$, with $\alpha = 0.1, 0.5, 1, 2,$ and 5, respectively. Each point represents an average over 10 clusters. It is seen that $M$ increases from 0 to 1 in a 2000 particles cluster for different $\alpha$. The error bar of $M$ in the cases of large value of $\alpha$ is larger than that for small $\alpha$, when $M$ changes from 0 to 1. It is also found that, the critical value ($\beta C$), from which $M$ increases from zero to unity, as shown in Fig. 6, is mostly dependence on the range of interactions (i.e., the value of $\alpha$). For small $\alpha$, the power–law interactions among particles are almost distance independent. The growth process is determined by the sum of magnetic interactions between all pairs of particles, which corresponds to small value of the critical ($\beta C$). As $\alpha$ increases, the power–law interactions become distance dependent, especially to the short-range interactions ($\alpha \geq 5$), the interaction between two particles decays rapidly with distance. The diffusion process and spin orientation are controlled only by the influence of the nearest neighbor particles, therefore, ($\beta C$) increases, and then reaches a saturated value with $\alpha$ further increases, as shown in Fig. 6.

On the other hand, the system energy of the magnetic DLA clusters grown with power–law interactions is studied in the...
follows. Fig. 7 gives the evolution of the energy $H/(|\beta C| \cdot N)$ per particle in units of the coupling parameter $\beta C$ for different $\alpha$, with $\beta C < 0$. It is clear that, for negative value of $\beta C$, the behaviors of $H/(|\beta C| \cdot N)$ vs. $\beta C$ are almost independence on the exponent $\alpha$. $H/(|\beta C| \cdot N)$ drops rapidly with the decrease of $\beta C$ and then approaches a steady value in the range of $\beta C = -50$ to $-400$. The energy behavior shown in Fig. 7 indicates that, for $\beta C < 0$, although the antiferromagnetic spin orderings shown in Fig. 1 are similar with different values of $\beta C$ and $\alpha$. However, there is a morphology transition [21] with $|\beta C|$ increases, since the diffusing particles would aggregate to the sites to reduce the system energy, due to the magnetic interactions among the particles in the cluster. With $|\beta C|$ further increases, the variation of $\beta C$ does not cause any major effect on the morphology [21]. In this case, the value of $H/(|\beta C| \cdot N)$ would not change anymore, as shown in Fig. 7.

For positive value of $\beta C$, the dependence of $H/(\beta CN)$ on $\beta C$ with different value of exponent $\alpha$ is shown in Fig. 8. Compared to the case of $\beta C < 0$ in Fig. 7, the effects of the magnetic interactions on the evolution of $H/(\beta CN)$ with $\beta C$ become important. For large value of $\alpha$ (i.e., $\alpha = 5$), as $\beta C$ increases, $H/(\beta CN)$ decreases slowly and then approaches a saturate value ($\sim -1.5$), which is related to the value of $\alpha$. However, no saturation of energy is observed for $\alpha = 0.5$ and $\alpha = 0.1$, and instead, a valley behavior exists in the energy curves, as shown in Fig. 8. With small value of $\beta C$, the variation of $\beta C$ does not cause any major effect on the morphology of cluster, which is likely DLA growth, due to the shielding effect of DLA model [21]. However, with $\beta C$ increases, the competition between the shielding effect and the power–law spin interactions changes, especially to the case of small $\alpha$. There is a morphology transition [21], a dense-branched cluster occurs for $\alpha = 0.5$ and $\alpha = 0.1$, corresponding to the lowest system energy in Fig. 8. With $\beta C$ further increases, the diffusing particle aggregates to the cluster before the system energy is lowest, therefore, the...
morphology of the cluster changes [21], and the energy $H/ (\beta C N)$ increases with $\beta C$, as shown in Fig. 8.

4. Summary

The influence of the power–law interactions on the magnetic DLA cluster has been studied by Monte Carlo simulations. It shows that, the evolution of spin distribution, magnetization and system energy of the cluster with the coupling $\beta C$ depends on the value of exponent $\alpha$, which corresponds to the range of spin interactions. These results may be useful to modeling and describing some similar experimental observations with long-range relevancy among them. For example, it can be used to simulate, or describe, the aggregation processes of multi-species systems, such as the aggregation of magnetic atoms or clusters on liquid substrates [22], where the magnetic atoms or clusters can diffuse and rotate on the liquid surfaces easily [22,23], and therefore, they can flip their magnetic moments freely with the magnetic coupling interactions among them. And also, the aggregation of the metal films on polymer substrates is another related example [24,25].

Acknowledgements

Financial supports from the National Natural Science Foundation of China (Grant no. 10574109), the Project of Zhejiang Provincial Science and Technology Department (Grant no. 2005C24008) and the Scientific Research Foundation of Zhejiang University of Technology, China (Grant no. 20060028) are gratefully acknowledged.

References