Diffusion limited aggregation of magnetic particles with exponential decreasing interactions in three-dimensional space

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Received 1 March 2014, www.cmnt.lv

Abstract

Using the Monte Carlo simulation, we investigate the three-dimensional fractal growth of a magnetic diffusion-limited aggregation (MDLA), which consists of magnetic particles interacting with an exponential potential βCe-αr. The cluster morphology, fractal dimension and magnetic susceptibility of this MDLA are analysed with respect to the range facto rα and the coupling energy βC. In the case of long-range ferromagnetic interaction, our results show that the cluster morphology grows to be a hexagonal symmetry as the coupling energy increases, which is different from the two-dimensional simulation. For a proper coupling energy, the fractal dimension takes the maximal value and the cluster morphology becomes more compact. In the case of short-range interaction, the critical value of the cluster specific magnetic moment is much larger than the simulation result in the MDLA with the interacting potential of power law.

Keywords: diffusion limited aggregation, magnetic particle, exponential decreasing potential

1 Introduction

Since the "diffusion limited aggregation" (DLA) model was introduced by Witten and Sander [1] in 1981, it has been extensively studied for the cluster fractal growth simulation and applied in various fields such as the viscous fingering [2], the electrochemical deposition [3] and the thin film growth [4]. Among the simulation efforts are DLA models that have been proposed to investigate the influences by different physical conditions on the cluster growth [5-10]. Hassan et al. [11] investigated a simple model, which described the aggregation kinetics of two-component (two-different-size) particles with stochastic self-replication. The particle anisotropy and particle shape are also discussed by Liu et al. [12] and Li et al. [13]. Vandewalle and Ausloos [14] introduced the spin degree of freedom for the aggregating magnetic particles. They studied the dependence of the fractal growth on the nearest neighbor coupling among the magnetic dipoles as well as the external magnetic field. Indiveri et al. [15] studied the morphology and symmetry of a two-dimensional cluster growing in the long-range interaction scenario with the power law potential $r^{-\alpha}$ (r is the distance between any two-grid points in the system, α is a positive constant). Furthermore, Xu et al. [16] studied the two-dimensional cluster morphology when the power law function interaction exists among magnetic particles. Their results show that, for the long-range ferromagnetic interaction and when βC takes appropriate values, the cluster morphology appears four-degree symmetry.

In many physical systems, the interaction potential appears the exponential function with respect to the distance between two objects. In ion chemistry, some atomic and molecular repulsive forces and hydrophobic forces decay as $e^{-\alpha r}$ [17]. In the direct electrochemistry of proteins, the reaction rate of the electro active substance on the electrode decreases exponentially with respect to the distance between the electron donor and acceptor [18]. In condensed matter physics moreover, the interactions among some electric dipoles and magnetic dipoles decay exponentially with their distances. In some correlative many body systems, the exponential potential $e^{-\alpha r}$ is often used as an approximation of the practical interaction [19]. Tomohiko et al. [20] using the Yukawa potential $r^{-1}e^{-\alpha r}$ to study the phase diagram of the Pd-Mn alloy. By means of the Fourier transformation.

This paper discusses the magnetic diffusion limited aggregation (MDLA) with magnetic particles diffusing in the three-dimensional space. The dipole-dipole coupling between magnetic particles is assumed to decay exponentially with the distance $\beta Ce^{-\alpha r}$. Using the Monte Carlo method, we study the fractal growth dynamics. The cluster morphology, the fractal dimension, and they are analysed with respect to the decay rate α and the coupling strength βC.

2 Modeling and simulation methods

Based on the well-known DLA model, the MDLA model introduces the spin degree of freedom [21], where each particle is a two-level system with $\sigma = +1$ standing for spin-up and $\sigma = -1$ standing for spin-down. The cluster is assumed to grow on a three-dimensional cubic lattice. The simulation algorithm is as follows:

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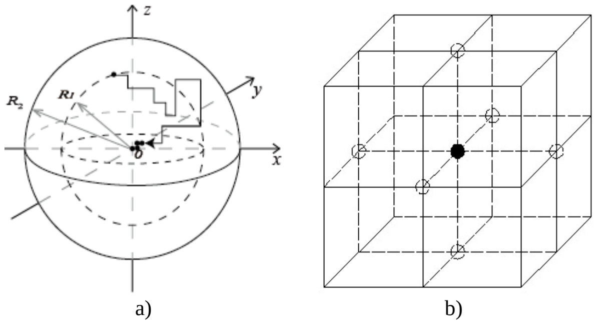


FIGURE 1 a) Illustration of the MDLA model and b) the six neighbor sites for a particle from the initial position diffusing

1) A seed particle with an initial spin state is placed at the centre of the cubic lattice (seed site).

2) Let the radius of the cluster aggregation is R_0, a diffusing particle with spin up or down is randomly generated on the spherical surface of radius $R_1 = R_0 + 20$, centred on the seed site.

3) The diffusing particle moves in the lattice according to the probability, which is determined by the change of the system energy with respect to the position and spin orient-tation. Considering the Ising coupling among the spins and their potential energy in the outer magnetic field, the dimensionless system energy can be defined as follows:

$$\beta E = -\sum_{\langle i,j \rangle} Jr_{(i,j)} \sigma_i \sigma_j - \sum_i \beta H \sigma_i \,, \qquad (1)$$
$$J\left(r_{i,j}\right) = \beta C e^{-\alpha r_{i,j}},\ \alpha \geq 0,$$

where $J(r_{i,j})$ is the coupling energy which is related to the distance $r_{i,j}$ between the particles i and j, βH is the outer magnetic field, and σ_i is the spin variable of the i-th particle. βC is the coupling strength related to temperature and α reflects the decay rate of the exponential function with the distance.

As illustrated in Figure 1, there are six neighbour sites where the diffusing particle from the initial site can move. The probability of moving to the m-th site is given by

$$P_m = \frac{\exp(-\Delta \beta E_m)}{\sum_{k=1}^{6} \exp(-\Delta \beta E_k)}, \quad m,k = 1,2,\cdots,6\,, \qquad (2)$$

where $\Delta\beta H$ is the energy difference induced by the change of the position and spin orientation. Using the roulette algorithm [22], we can select the location of the particle diffusion and spin orientation.

If the particle diffuses to the site connected to the condensed cluster, the particle will adhere to the cluster, and the spin orientation of the particle will be frozen. If the particle moves outside the spherical surface of radius $R_2 = R_0 + 30$, centred on the seed site, the particle disappears. In either case, one returns to the second step for another diffusing particle. The diffusing processes are repeated until a fractal cluster of N particles is formed.

3 Results and discussion

As an extension of the classical DLA model, the energy difference in the MDLA model is jointly determined by the diffusing particle's position and spin orientation. By tuning the parameters βH, βC and α, we can simulate the growth process of condensed clusters in the situation of different magnetic fields and temperatures. For simplicity, we consider the case of magnetic field strength $\beta H = 0$ in this paper. The spin of the seed particle is set to be spin-up. The two spin states, up and down, are illustrated by blue color and red color respectively. According to the energy Equation (1), we can know that, when βH and βC are close to zero, the energy difference before and after the particle diffusion is approximately zero. Therefore, the probabilities of the particle diffusing to different nearest neighbors are same. The motion is approximated to the uniform random walk process, and the formed cluster morphology is similar to the DLA model.

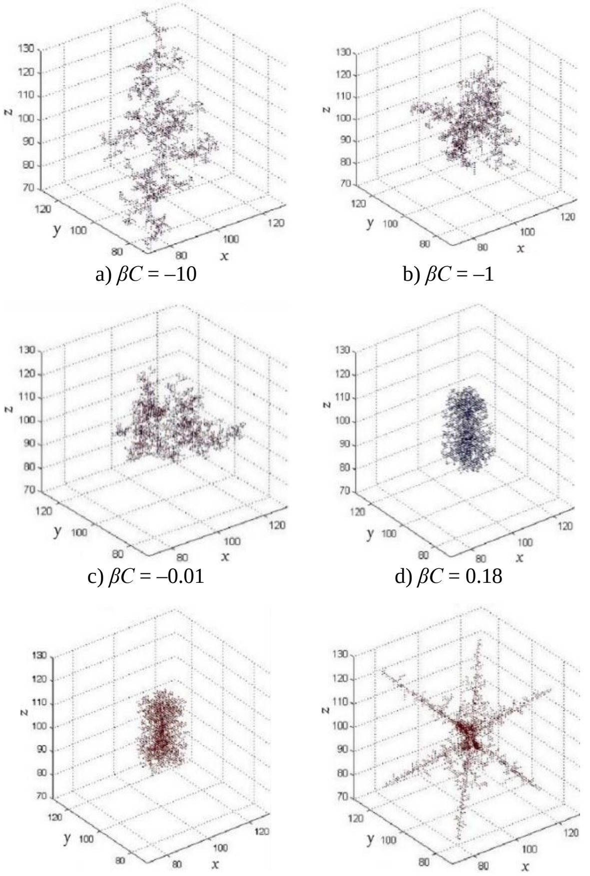
3.1 FRACTAL MORPHOLOGY OF THE LONG RANGE MAGNETIC INTERACTION SYSTEM

When the parameter α is small, the coupling energy between the magnetic particles damps slowly with their distance, and hence there is a long range interaction between the magnetic particles. Figure 2 shows the cluster morphologies with fixed $\alpha = 0.2$ and various $\beta C = -10, -1, 0.01, 0.18, 0.22, 200$.

Figures 2a and 2b show that when βC is negative, the cluster grows by the antiferromagnetic way. The cluster morphology becomes looser as $|\beta C|$ increases. The spin states of the magnetic particles present a regular crosswise distribution as shown in Figure 3a.

When βC is positive, the cluster grows by the ferromagnetic way. With the increasing βC, the cluster morphology becomes more and more regular as a six-degree symmetry structure distribution. As shown in Figure 1(f), the six-degree symmetrical structure corresponds to simple cubic lattice structure. In fact, the similar structure of six-degree symmetry widely exists in the systems (e.g., $\alpha = 0.1, 0.25, 0.3, 0.4$) of long range magnetic interactions.

When βC varies from 0.1 to 0.5, influenced by the random Brownian walking, the spin distributions of dominant up and dominant down appear alternately as shown in Figure 2c and 2d. However, when βC takes values greater than 0.8, the spins in the cluster are completely magnetized to the up state like the seed particle. This means that the force of the cluster imposing on the diffusing particle is increasing. The diffusing particles take the same spin states for the lower system energy. The certainty factor of the spin interaction plays a major role; while the effect the random factor is weaken.

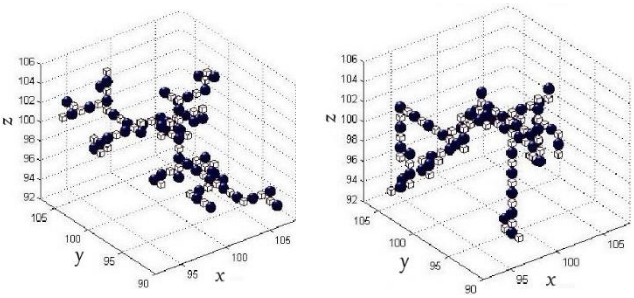


a) $\beta C = -10$ b) $\beta C = -1$

c) $\beta C = -0.01$ d) $\beta C = 0.18$

e) $\beta C = 0.2$ f) $\beta C = 200$

FIGURE 2 The cluster morphologies for various βC but fixed $\alpha = 0.2$



a) $N = 200$, $\alpha = 0.2$, $\beta C = -50$ b) $N = 200$, $\alpha = 1$, $\beta C = -50$

FIGURE 3 The morphology of aggregates

3.2 FRACTAL DIMENSION OF THE LONG RANGE INTERACTIONS SYSTEM

In Figure 4, the fractal dimension of the cluster is plotted with respect to βC. In the case of antiferromagnetic growth, as $|\beta C|$ increases, the fractal dimension D_f gradually reduces to about 1.79. When βC reduces to - 100, the cluster no longer maintains the DLA fractal structure, but shows a broadband-like morphology.

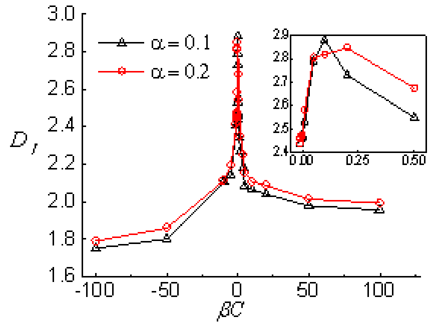
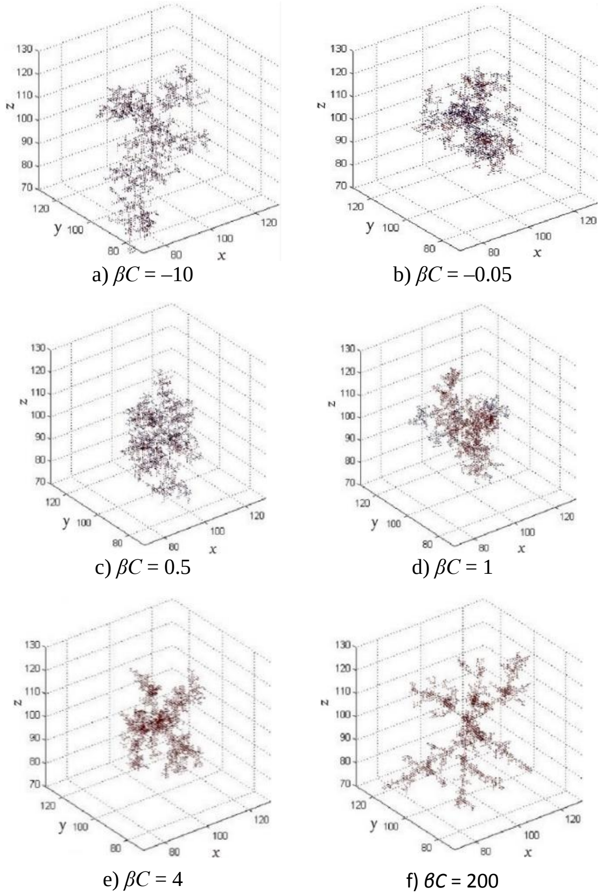


FIGURE 4 Aggregation clusters fractal dimension of different parameter βC when $\alpha = 0.1, 0.2$

In the case of $\beta C = 0$, clusters of fractal dimension is about 2.47. In the case of ferromagnetic growth, the value D_f of the cluster changes significantly with the increase of βC. Especially for the system of $\alpha = 0.1$, the value D_f has a maximum peak value of 2.88. In the system of $\alpha = 0.2$, D_f, also has a maximum peak close to 2.84. However, as βC continues to increase, the fractal dimension decreases sharply. As shown in Figures 2d and 2e, the morphologies of the clusters are relatively tight, and the system energies are the smallest, which means the systems are stable. With $|\beta C|$ increasing, the morphology varies similarly to the case of $\alpha = 0.1$, except that the value D_f drops relatively slow.



a) $\beta C = -10$ b) $\beta C = -0.05$

c) $\beta C = 0.5$ d) $\beta C = 1$

e) $\beta C = 4$ f) $\beta C = 200$

FIGURE 5 The the cluster morphology in different parameter βC but fixed $\alpha = 1$

3.3 FRACTAL MORPHOLOGY OF THE SHORT RANGE MAGNETIC INTERACTION SYSTEM

When the parameter α is large, the coupling energy between the magnetic particles damps quickly with their distance, and hence the magnetic particles have the short-range interactions with each other. Only when closing to the aggregation cluster, does the diffusing particles can be affected by the cluster heavily. Figure 5 shows the growth morphology of the clusters with $\alpha=1$ and $\beta C=-10,-0.05,0.5,1,4,200$.

Figures 5a and 5b show that, when βC is negative, the clusters grow in the antiferromagnetic way. Similar to the long range interaction system, as $|\beta C|$ increases, the morphology of aggregation cluster is more and more loose, and the spin state presents a crosswise distribution as shown in Figure 3b. But under the long range interaction system, the morphology gets sparse relatively faster.

When βC is positive, aggregation clusters grow in the ferromagnetic way. Unlike the long rang interaction system, the cluster morphology does not vary obviously and won't appear the six degrees of symmetrical structure even though βC is very large. For the larger $\alpha(\alpha>1)$, the branch tips of the cluster are forked. The cluster tends to be unstable and the morphology is not compact like that in Figure 2b any more. The reason is that, in the short range interaction system, when the diffusing particle is far away from the cluster, the influence made by the cluster to the diffusing particle is approximate to zero. Only when the diffusion particles move close to the aggregation clusters, does the magnetic interaction between the particles has a significant impact. However for the long range interaction system, from the beginning of its movement, the diffusing particle is affected by the cluster, and when βC takes appropriate values, the magnetic particles agglomerate more closely so that the cluster energy will be less and the system will be more stable.

When $\beta C<1$ the spin-up particles and the spin-down particles appear in the aggregation cluster at the same time. But as βC increases, the number of spin-up particles increases. When $\beta C>4$ all condensational particles are magnetized to spin-up state. In short-range interaction systems, the value of βC that magnetizes all aggregation clusters to spin-up state is much larger than that in the long range interaction systems.

3.4 THE FRACTAL DIMENSION IN THE SHORT RANGE INTERACTION SYSTEMS

Figure 6 shows the cluster fractal dimension curve with respect to βC when $\alpha=1,3$. We can see that when βC is negative, the cluster grows in the antiferromagnetic way. when $\alpha=1$ with $|\beta C|$ increasing, the fractal dimension decreases gradually to about 2.13. When $\alpha=3$, as $|\beta C|$ increases, the fractal dimension of clusters decreases gradually to about 2.4. When βC is positive, the cluster grows by ferromagnetic way. As βC increases, when $\alpha=3$, $100>\beta C>-100$, D_f, the fractal dimension distributes between 2.4 to 2.58 and does not appear the maximum peak that similar to the maximum peak in the long-range interaction systems. When βC is smaller, the value of D_f is about 2.48, and it is similar to the classic DLA model. With βC increasing, D_f, decreases gradually and tends to a stable value about 2.4. For short range interaction system, magnetic particles near the aggregation clusters determine direction of spin particles, therefore, regardless of ferromagnetic or antiferromagnetic growth way, it has a small influence to the cluster morphology, and the difference of its fractal dimension change is not obvious.

3.5 SPECIFIC MAGNETIC MOMENT

In order to study the evolution of the spin state under different forces, we analysed the dependence of the specific magnetic moment M of aggregation clusters on the parameter βC. The specific magnetic moment M of the cluster is the ratio between the total spin and the total number of the particles, where the total spin indicates the difference between the numbers of spin-up particles and the spin-down particles.

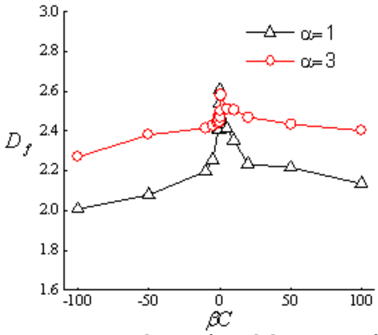


FIGURE 6 Aggregation clusters fractal dimension of different parameter βC when α = 1;3

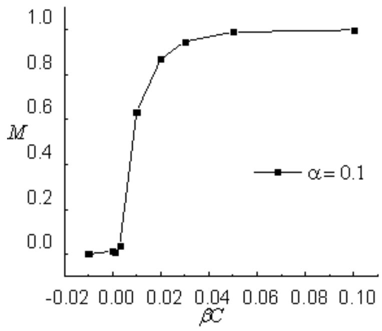


FIGURE 7 The curve of M changing with βC when α = 0.1

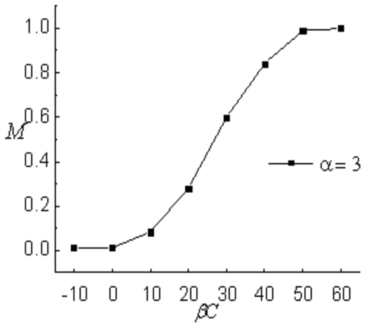


FIGURE 8 The curve of M changing with βC when α = 3

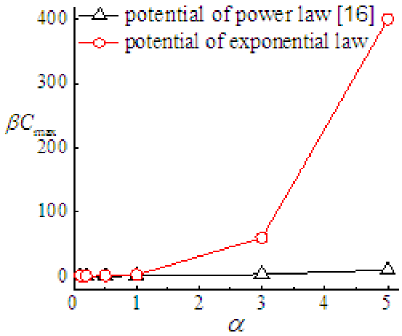


FIGURE 9 The curve of the critical value βC_{max} changing with different forcing process parameters α

As shown in Figures 7 and 8, in both cases of the long range interaction and the short range interaction, when βC is negative, the specific magnetic moment of aggregation clusters decreases and tends to 0 with $|\beta C|$ increasing. In the case of long range interaction $\alpha = 1$, the specific magnetic moment increases rapidly with βC increasing, and to the saturate value 1 as βC increases beyond 0.05. In the case of short range interaction $\alpha = 3$, the specific magnetic moment increases slowly with βC increasing, and when βC goes beyond 60. All of the aggregation particles are magnetized to spin-up state i.e., the specific magnetic moment $M = 1$. In the short-range interaction force, although the particle spin- flip probability is small, but once the spin flip, subsequent particle also will spin flip, resulting magnetization fluctuation phenomena.

For a given interaction range factor α, one can always find the threshold βC_{max}, which leads to the complete magnetization $M = 1$. Figure 9 shows the magnetization threshold βC_{max} as a function of the range factor α. In the case of long range interaction, the interaction between the particles did not change significantly with their distance, the magnetization threshold βC_{max} various slowly with the range factor [16]. As α increases to the short range interaction cases, the interaction strength between particles decays rapidly with their distance. The value of βC_{max} under the power law interaction is significantly greater than that under the exponential interaction. The influence that βC made to the specific magnetic moment in the power law interacting particles is far less than that made to the specific magnetic moment of exponential law interacting particles.

4 Conclusion

Using the MDLA model and assuming that the magnetic interaction force between the particles decays exponentially with their distance, we simulated the dynamic behavior of cluster fractal growth for different physical parameters. When the cluster grows in the antiferromagnetic way, the spin states of magnetic particles under different forces are in a crosswise distribution. Along with the decrease of the parameters of α and βC, the morphology of aggregation clusters gets more sparse, the fractal dimension decreases continuously, and the specific magnetic moment of aggregation clusters tends to be zero. When the cluster grows in the ferromagnetic way, for long range interaction systems, the cluster morphology and fractal dimension change significantly with the physical parameters. The cluster morphology evolves to regular six-degree symmetric structure from the ordinary DLA morphology, and there are also dense forms appear in the middle range. The specific magnetic moment M increases rapidly from 0 to 1 as the parameter βC increases. For short-range interaction systems, the cluster morphology and the fractal dimension change slowly with the physical parameters. Moreover, the compact structure and six-degree symmetric morphology does not appear. The specific magnetic moment M also increases slowly from 0 to 1 as the parameter βC increases. This conclusion provides a reference for explaining the related phenomenon of physics experiments and studying the fractal growth mechanism of magnetic particles, etc.

Acknowledgments

This research was supported by the National Natural Science Foundation of China (Grant Nos. 61273088, 11271194 and 11201264).

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