The effect of seed geometry and size on the mechanism of the pattern formations in two-dimensional space by Monte Carlo simulation

M. BAYIRLI*, H. KOCKAR, Z. MERDAN[a]

Department of Physics, Science and Literature Faculty, Balikesir University, Balıkesir, Turkey

[a] *Department of Physics, Science and Literature Faculty, Gaziosmanpaşa University, Tokat, Turkey*

The effect of the seed geometry and size on the pattern formation mechanism in two-dimensional space was investigated by Monte Carlo (MC) simulation using the fractal concept and particles density. The patterns obtained from the square seed has symmetrical main brunches whereas the circle seed patterns pose the denser and higher number of brunches with the increase of the dimension of the seed, and hence they have both long-range correlations. The critical exponents, α and the fractal dimensions, D_f were computed using the power-law. The results were compared with a model based on the diffusion-limited aggregation (DLA) obtained by MC. It is seen that the morphology of the patterns is greatly affected by the geometry and size of the seeds. Therefore, in order to quantify the change of D_f with geometry of the seeds, the fractal dimension function, $D_f (l)$ and $D_f (r)$ for length of the square and circular seeds were introduced, respectively. The results are expected to provide an expansion of the DLA model in terms of geometry and size of the seeds.

(Received April 29, 2008; accepted May 21, 2009)

Keywords: Monte Carlo simulation, Diffusion-Limited Aggregation, Seed, Numerical calculation

1. Introduction

The structures of aggregates strongly depend on the dynamics of growth process. A large number of theoretical analysis and computer simulation models have been carried out to investigate the relationship between geometry and growth mechanism of patterns [1-4]. The Laplacian growth model based on the Diffusion-Limited Aggregation (DLA) model that can be simulated by Monte Carlo (MC) simulation provides an approach to these phenomena. Thus, the DLA presents a prototype of pattern formation of diffusive systems, including electrodeposition, colloid aggregation, etc. [3-8]. The parameters of the sticking probability kinetics [4, 6], surface diffusion [9], and many particle iterations [10] were added to the DLA model in order to study more realistic physical systems using the DLA process.

The standard DLA model simulates the growth of a pattern by considering the random walks of a particle on one pixel square lattice containing a seed. If the mobile particle encounters the seed in the first square seed, it ceases to sit there. Otherwise it continues to move until it finds another particle to stick to each other. Successive walkers repeat this process. The fractal pattern formation can be produced by MC simulation [2, 4].

The crystal pattern is generally presumed to begin from a single square immobile seed in DLA simulations, but it is not always true in reel systems. To our knowledge, the shape of the geometric structure of the seed has not been taken into consideration in the DLA model but Deepak at al [11] indicated the segregation of crystal growth patterns of two square seeds using the fractal geometry and stick probability [4, 9].

The aim of this study is to investigate the effect of the seed geometry and size on the pattern formation mechanism. The geometry of the seeds was selected as square and the circle in shape. The patterns were simulated by MC technique based on DLA model. It is found that the results of the geometrical parameters lead to an extension of the DLA models and hence expected to have a wide range of application in the field of simulation of reel systems. The fractal dimension function, $D_f (l)$ for length of the square seed and $D_f (r)$ for the circular seeds were also introduced, respectively.

2. Model and simulations

The MC model is used to simulate the patterns grown around the square and the circular seed based on DLA in order to compare the geometrical parameters of critical exponents (α) and fractal dimensions (D_f). To DLA model, the MC algorithm was as follow: The particle walks on continuous in lattice and moves a distance of one length unit for each MC step. A random walker is introduced and moves on the lattice with the equal probability of ¼ of walking in each of four directions at each MC step until it reaches the occupied site at which one pixel seed, and it sticks with probability one [3, 4]. In the standard DLA patterns, to verify the above algorithm, a seed is occupied on a square lattice of one pixel, and the typical simulated pattern is shown in Fig. 1(a). In this study, a series of the square seed and circular seed lattices were simulated in various pixels, respectively. The typical of patterns simulated in 40 pixels for the length of the square and the radius of the circle were presented in Fig. 1(a) and Fig.1 (b), respectively.

3. Results and discussion

Numerical simulations are performed on the finite square lattice (*LxL)* using MC method based on DLA model. The length of the particles is chosen as one lattice unit of one pixel for the standard DLA model, and 40 pixels for the square and circular lattice. The occupied fraction of the aggregates is given by $\rho=n/L^2$, where *n* is the total number of particles. *L* is chosen to be 400 for all simulated patterns.

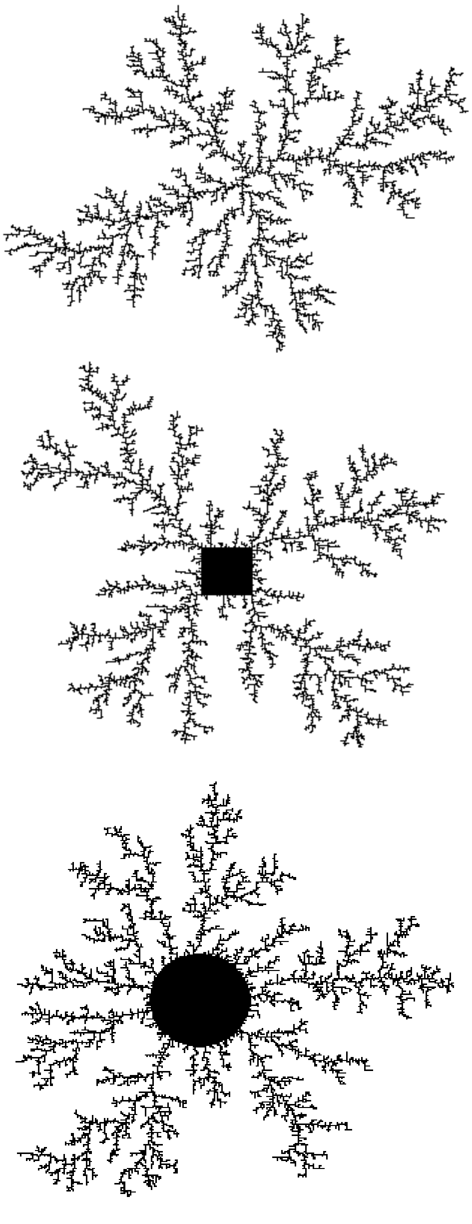

Fig. 1. Typical morphologies of the crystal patterns of (a) l=1 pixel seed for standard DLA, (b) l=40 pixels for square seed and (c) r=40 pixels for the circular seed.

The length (*l)* of square seed are arbitrary chosen as from 1 to 350 lattice units, and the radius (*r)* of the circle seed are varied from 1 to L/2 in the finite square lattice in two-dimensional space. They are shown in Fig.1. In Fig. 1(a), Typical DLA patterns are observed and have five main brunches and some sub-brunches on them. Fig.1 (b) shows the less main brunches with sub-brunches and denser structure compared to the DLA pattern. Main brunches are occurred from the corner of the square seed of 40 pixel but no main brunches at the edge are obtained due to the symmetry of the square lattice. In the case of Fig. 1(c), the number of main and brunches increased with the increase of sub-brunches having the densest structure. Just as the radius of the circular seed increases, the numbers of the main branches increase in the environment of the circular seed.

All patterns simulated in this study have long-range order. The patterns in Fig. 1(b) and Fig. 1(c) have less number of sub-brunches and long-range deformation compared to the standard DLA growth in Fig. 1(a) due to the size of the seeds. The thickness of the branches and sub-brunches are different. Bigger size of the seed makes the brunches thicker and also the degrees of the thickness were also affected by the geometry of seed. To do the pattern simulation in a much larger-scale as in case of 40 pixel square and circular seed pattern, the number of branches would be increase and, accordingly the branches would become relatively thicker for the around circle deposit seeds.

The geometrical parameters of the simulated patterns were computed. The static property can be reflected by fractal dimension (D_f). D_f of patterns is calculated by the box-counting method. The method is used to study the random set in a lattice. The density-density correlation function, *C(r),* was used to detect the fractality of the crystal pattern as defined in [1, 2, 4]. The correlation function is given by;

$$C(r) = \frac{1}{N}\sum_{r'} \rho(r + r')\rho(r') \qquad (1)$$

where *N* is the number of particles in the same clusters and ρ is the local density. This equation gives the probability of finding a particle at the position $\boldsymbol{r} + \boldsymbol{r}'$, if there one at $\boldsymbol{r}'$. *r* is the first particle distance from the selected particle, and $\boldsymbol{r}'$ is the distance of the other particles from *r*. This equation gives the relationships among the particles in the patterns.

The *C(**r**)* was calculated and plotted against *r* in the logarithmic scale as seen in Fig.2. Since the patterns are fractals, the shape of the straight line was fitted to the data on logarithmic plot. This indicates that the density-density correlation function within the patterns decays according to power law. In all cases, the rapid decreases in *C(**r**)* at high ***r*** values are due to the long size of patterns. The differences in the *C(**r**)* are due to the geometry of the seeds. In the circular seed, the slope of the pattern has the smallest fitted line, and followed by the square seed and then the standard DLA seed in Fig. 2. The reason for that is the distribution of the number of particles in square and circular seeds is bigger then the seed of the standard DLA pattern.

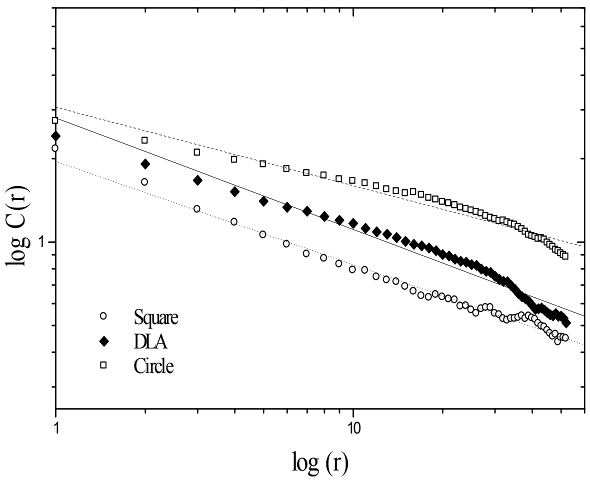

*Fig. 2.) Logarithmic plot of density-density correlation function C(**r**) as a function of distance **r** for l = 1for Standard DLA seed, l = 40 for square seed, r = 40 for circle seed.*

In addition to the simple power law of $C(\mathbf{r}) \sim \mathbf{r}^{-\alpha}$, α is obtained from each straight line and summarized in Table 1. The lowest α of 0.236±0.004 was calculated for the pattern of circular seed for the radius seed, r=40. Fractal dimension (D_f) corresponds α with $D_f = \alpha+2$. The D_f values were computed for each of the patterns. In the standard DLA pattern, D_f is 1.660±0.004 and is around 1.70 in [2,4].

Table 1. Critical exponents for patterns r: radius of the seed, l: length of the square seed.

Seed	Length or radius of the seed	Critical exponents, α
Circular	r=40	0.236±0.004
DLA	l=1	0.340±0.005
Square	l=40	0.392±0.006

In order to quantify the change of D_f with geometry of the seeds, the fractal dimension function, $D_f\,(l)$ and $D_f\,(r)$ for length of the square and circular seeds were introduced, respectively. They are computed and plotted in Fig.3. Just as one expects to reach an asymptotically non-fractal patterns, the $D_f\,(L)$ become a finite value 2 as $l \rightarrow L$. In Fig.3, it can be seen that the $D_f(l)$ has slower increase then the $D_f(r)$ since the brunches can only grow in the corner of pattern of square seed, which has less brunches.

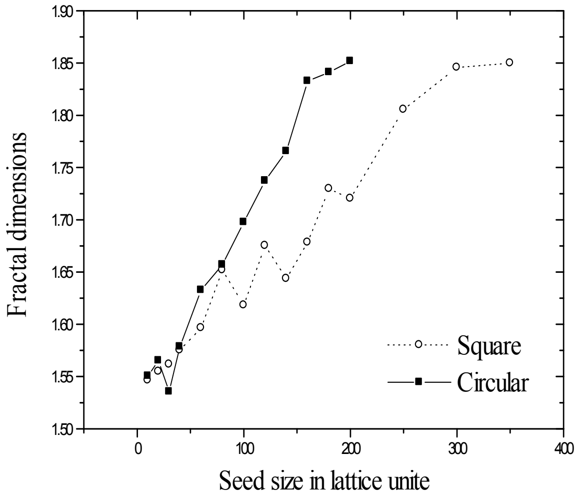

Fig. 3. D_f versus the length, l of the square seed and the radius, r of circular seed. The $D_f(l)$ and $D_f(r)$ were obtained from the fitted line using nonlinear regression.

Nevertheless, the approach to the initial parameter was estimated as the functions of $D_f(l)$ and $D_f(r)$ using the non-linear regression method. The following equations of $D_f\,(l)$ and $D_f\,(r)$ are obtained by fitting data for each patterns in Fig.3.

$$D_f(l) = D_0 + Al^{\mu} \tag{2}$$

and

$$D_f(r) = D_0 + Br^{\delta} \tag{3}$$

where μ and δ are the correlation exponents for the $D_f\,(l)$ *and* $D_f\,(r)$ are obtained from non-linear regression in Fig. 3 , respectively. A and B are constants, and D_0 is defined as the D_f of the standard DLA pattern.

The μ is computed as 0.968±0.194 while the regression coefficient, R=0.981 for the square seeds. The other exponent δ is 1.082±0.156 with the regression coefficient, R=0.987. It can be said that μ and δ depend on the geometry and size of the lattice seeds.

6. Conclusions

The mechanisms of the patterns grown around the different geometry and size of the seeds in two-dimensional space have been investigated by using a MC simulation based on DLA model. The effect of the seed geometry is studied by simply changing the shape and size of seeds. The patterns obtained from the circular seeds have symmetrical and more main brunches whereas the square seed patterns have the less dense brunches with the increase of the dimension of the seed. The α and the D_f were computed using the power-law. These results were compared with the simulated model based on the DLA obtained by MC simulation. It is seen that the morphology of the patterns is greatly affected by the geometry and size of the seeds. Therefore, in order to quantify the change of D_f with geometry and size of the seeds, the fractal dimension function, $D_f\ (l)$ and $D_f\ (r)$ for length of the square and circular seeds were introduced, respectively. The results are expected to provide an expansion of the DLA model in terms of geometry and size of the seeds. Therefore, it is anticipated that this approach would generate a wide variety of patterns under reel pattern conditions.

Acknowledgements

This work is partly supported by Balikesir University, Turkey under Grant no BAP 2006/26.

References

[1] P. Meakin, Fractals, Scaling and Growth far from Equilibrium, Cambridge University Press, Cambridge, 1998.
[2] T. A. Witten and L. M. Sender, Phys. Rev. Lett. **47** 1400 (1981).
[3] P. Jenses, A. L., Barabasi, H. Larralde, S. Havlin and H. E. Stanley, Phys. Rev. B. **50,** 15316 (1995).
[4] T. A. Witten, L.M. Sander, Phys. Rev. B. **27,** 5686 (1983).
[5] D. G. Grier, D. A. Kessler and L. M. Sender, Phys. Rev. Lett. **59,** 2315 (1987).
[6] P. Meakin, Phys Rev. A. **27,** 2616 (1983).
[7] M. Bayirli, Physica A. **353,** 1 (2004).
[8] R. F. Xiao, J. I. D. Alexander, F. Rosenberger, Phys. Rev. A **38,** 2447 (1988).
[9] P. Meakin, Phys Rev. A. **153,** 1 (1998).
[10] D. N. Bankar, P.M. Gade, A.V. Gade, A. V. Limaye, A. G. Banpurkar, Phys. Rev. E. **75,** 051401 (2007).
[11] J. Nittmann, H. E. Stanley J. Phys. A. **20, L,** 981 6 (1987).

*Corresponding author: mbayirli@balikesir.edu.tr, mehmetbayirli@yahoo.com