Off-lattice Simulation of the Fractal Growth with Attractive Radial Drift and Mobility

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In the perfect off-lattice DLA model of the fractal growth the centre-attractive drift factor and mobility of particles are introduced. Simulation indicates variation of fractal patterns and their characteristics depending on these new factors. Noticeable effects of the drift factor upon fractal dimension, growth efficiency and frozen zone are shown. The mobility behaves in the competitive manner with the drift. The combination of drift and mobility is considered as analogs of potential and kinetic energies of particles.

Key words: fractal growth, the diffusion limited aggregation.

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1 Introduction

Fractal growth models attract remarkable interest last 10-15 years in physics, chemistry and other fields in connection with applicability to many phenomena where random initial conditions result in formation of objects with explicit spatial self-similarity. For example, electrochemical deposition of metals is known to lead at the certain conditions to different fractal patterns [1]-[10]. Fractals reveal a number of non-trivial properties (optical, catalytic, electrochemical, etc.) [11]-[16] those are associated with peculiarities of both local structures of fractals and their global self-similarity which can provide a correlated behaviour of particle contribution in properties of aggregates. Recently [17] we reported about formation of fractal structures in titanium thin films with small silver particles by the process of the selective cathodic silver deposition [18]. This system with fractal aggregates which consist of 10–100 nm silver particles reveals also the pronounced change in kinetics of redox-processes as compared with non-fractal analogous systems. In the present work we construct the model of fractal growth on the basis of the standard diffusion limited aggregation (DLA) of particles in two dimensions including two additional parameters: (i) particle attractive radial drift, i.e. increased probability to move in the direction of some centre (attraction); (ii) mobility of particles which relates to the regulation of the particles’ ability to respond upon the drift effect. It can make disorder in the resulting aggregate, while the drift effect, evidently, aspire to more ordering of growing clusters. Similar parameters were considered in some models earlier [19]-[21], however, the full off-lattice simulation with drift and mobility is analysed here for the first time (for our knowledge).

It should be noticed that within the framework of lattice models (more distributed in literature [22] any inclusion of the two above features (both drift and mobility) is problematic. A discreteness of lattice models is known to lead to artefact ordering of fractals due to lattice geometry. These main features of our model (drift and proper mobility) can be associated, respectively, with the attractive force to a centre of growth and kinetic energy of particles which are the universal characteristics for any particle-aggregation phenomenon. In the context of lattice models the potential field effect upon DLA
was considered in [23]-[26].

2 Model

The main features of the model used for construction of the calculation algorithm are depicted in Fig. 1. A particle is created at some radius from the seed (the centre of growth) and walking in arbitrary direction by jumps to some point located at the distance $M$ from the creation site, where the $M$ value characterizes the mobility of a particle. Thus, in general in the off-lattice model

$$(x_{i+1}, y_{i+1}) = \text{Random}(x_i, y_i),$$

(1)

$\text{Random}$ is a discontinuous function of angle $\alpha$ for radius-vector $(x_i, y_i)$ and distance $\sqrt{x_i^2 + y_i^2}$.

$$(x_{i+1}, y_{i+1}) = M \cdot \text{Random}(x_i, y_i)(1 \pm \frac{P_{drift}}{\sqrt{x_i^2 + y_i^2}}),$$

(2)

where $\pm$ corresponds to repulsion from the centre ($x=0, y=0$) or attraction to it, respectively. We restrict ourselves here by the case of attraction. $P_{drift}$ is drift factor, $P_{drift} = \text{const} : 0; 0.1...5$; and the mobility used for each particle jump $M = P_M \cdot M_{max}$, where $M_{max} < 50$ and $0 < P_M < 1$.

A drift contribution to the random walking can be present as

$$\frac{P_{drift}}{\sqrt{x_i^2 + y_i^2}} \sim \frac{1}{R_i},$$

(3)

where $R_i = \sqrt{x_i^2 + y_i^2}$ is current distance to the centre $(0,0)$.

The simulation for each trial was stopped when the diameter of aggregate attains 500 particles. This value is sufficient for statistical analysis and requires reasonable time for performing of several trials with same initial parameters.

Such model can be adopted also to the 3-dimensional case since we use two coordinates $x$ and $y$ on equal footing, but it requires much more CRU time for calculations. The present two-dimensional simulation was carried out with RS6000 workstation, and the generation $1000 \times 1000$ output sets required tens of hours for each trial.

3 Results of Simulation and Discussion

The overall picture of typical aggregates is presented in Fig. 2 for selected values of drift factor and mobility. Under small values of these parameters we obtain usual DLA-fractals (it is shown by the left top corner pattern (1)). The drift factor used and the mobility value are given in dimensionless units so, $M = 1$ and $P_{drift} \ll 0$ correspond to usual DLA-fractals. Then, we see from Fig. 2 that the drift equals to 0.01 is essential upon the outlook of patterns. The increase of $P_{drift}$ effectively makes more

FIG. 1. The sketch of the model used for simulation

When this particle appears to be close to the centre or the seed of the growing aggregate it binds into it. The drift factor is introduced as increase of probability to move to the centre as compared with random Brownian motion. The mobility is given by the value of jumps. It varies also by a random way, and jumps may be inside the interval from zero to $M_{max}$. 

dense aggregates, however, no any concentration of particles to the centre appears, the fractals retain general uniformity in particle density. The value of $M$ must be considered in this model with respect to overall size of aggregation area ($1000 \times 1000$) and taking into account the difference with the standard DLA (when $M = 1$). We see that noticeable effect begins from $M > 10$, but even $M = 50$ produces weakly noticeable changes in the case of small drifts, but under big drifts the mobility acts against the drift factor affecting the density of particles. Thus, $P_{\text{drift}}$ has the independent significant contribution to the resulting fractals, whilst the mobility appears to be remarkable together with the drift.

From the resulting patterns of aggregates we calculated the quantitative parameters those characterized the fractals, and they are depicted in Fig. 3–5. We consider the following parameters: (i) fractal dimension, $D_f$, which was determined by the standard method through $\log(N) - \log(R)$ curves; (ii) the frozen zone, i.e. the area which leaves without new particles under growth; (iii) the growth efficiency, $N_{\text{created}}/N$, the relationship of the full number of particles created to the number of particles in the fractal (joined to the aggregate during the growth). All points on the plots were obtained in the result of averaging several (not less than 3) full trials with equal initial data.

From the data on $D_f$ we can conclude that the drift effect retains the fractal character of aggregates and increases $D_f$ without attaining 2 under the range of $P_{\text{drift}}$ studied. $P_{\text{drift}} = 5$ is rather high value according to the effects observed, and the simulation with larger $P_{\text{drift}}$ gave no qualitatively new results. Some saturation of $D_f$ vs $P_{\text{drift}}$ is observed for small mobilities (Fig. 3a). Also, the large drift factor results in certain value of fractal dimension (about 1.88) that is weakly dependent on $M$ (Fig. 4a).

Plots of the frozen zone vs $P_{\text{drift}}$ (Fig. 3b,4b) show that all aggregate become active in the growth with the increase of the drift, while the mobility has no such essential effect upon the frozen zone, and some its decrease occurs. The latter is rather unexpected a priori, since $M$ is the measure of ability of a particle to penetrate to remote points. Hence, for this model the mobility (associated with the kinetic energy of particles, see below) is the factor of dynamics rather than of final state. For example, the time consumed for the full growth is rapidly decreasing function of $M$ (not shown in Figures).

The growth efficiency also behaves in different way for $P_{\text{drift}}$ and $M$-dependencies (Fig. 3c,4c). It fast decreases with the rise of $P_{\text{drift}}$, but in the case of high mobilities this effect is less and approaches unity, i.e. the high 'aspiration to fall to the centre' produces the growth without fruitless creations and motion. In contrast, under high mobility all high-drifted fractals are distinguished by this parameter, while under low mobility low-drifted ones have remarkably different growth efficiency. Thus, smallest and largest values of the drift factor (among range studied) show weak mobility dependencies. It is interesting point about mutual effects of these factors: mobility acts in the medium range of $P_{\text{drift}}$. 

![Fractal patterns example](image-url)
The similar tendency appears also in Fig. 3c for the growth efficiency vs $P_{\text{drift}}$, we see more difference in the medium range (near $P_{\text{drift}} = 0.1$ there is a maximum difference).

The number of particles joined to the final fractals enters the range tens and hundreds of thousands and noticeably grows with the increase of the drift factor (Fig. 5a). That is quite trivial observation, and it results in higher density of particles and slightly higher value of $D_f$. However, the mobility effect upon the number of particles is not trivial and has decreasing (big $P_{\text{drift}}$) and increasing (small $P_{\text{drift}}$) parts. The high mobility makes less differences in this parameter for different drifts (Fig. 5b). Thus, again it acts in competitive manner with the drift factor.

The general overview of the simulation results presented above supports possible direct association of the two main factors affecting the growth of DLA fractals with realistic characteristics of the moving particles - potential and kinetic energies. The first is associated with the drift factor, and the second one is connected with the mobility. Potential energy of the particles can appear here due to the centre-attracting field which provides the drift, and the kinetic energy is the measure of the particle speed. Such associations support observed competitive action of these factors upon fractal parameters. It is well known that they have such property in mechanics, and occurrence of external field allows to resolve different energies of moving particles (e.g. mass-spectrometry). In this context, the less expressed effect of the mobility for largest drifts (associated with high external fields providing potential energy of particles) can be understood similar to usual mechanical or electrodynamic analogies. Thus, possible applications of the model considered in the work...
FIG. 5. The effect of the drift factor (a) and the proper mobility (b) upon number of particles in the fractals in the result of aggregation during certain time.

is in the selective electrochemical deposition of metals, namely, field effect upon metal ions and their mobility are the main factors of this process.

4 Conclusions

1. The full off-lattice 2-dimensional model of fractal aggregation is studied for the first time with two additional factors: drift and mobility.

2. The drift (modelling attraction to the centre) results in increase of $D_f$ with change from explicit fractal to more dense aggregates. Under high drift factors the fractal dimension conserves with the growth and the frozen zone tends to 1. The effect of mobility appears to be both similar to a drift (under small drift factors) and opposite to it (at high drifts). It is most evident under medium values of the drift factor also.

3. Inclusion of drift factor and mobility in the DLA model preserves the fractal character of aggregation with self-similarity. These two factors can be associated with the potential and the kinetic energy of particles.

References