Effect of drift on segregation in two-component diffusion-limited aggregation

Takashi Nagatani
Departament de Quimica-Fisica, Universitat de Barcelona, Diagonal 647, E-08028 Barcelona, Spain and College of Engineering, Shizuoka University, Hamamatsu 432, Japan

Francesc Sagues, Josep Claret, Francesc Mas, Pedro Pablo Trigueros, and Jordi Mach
Departament de Quimica-Fisica, Universitat de Barcelona, Diagonal 647, E-08028 Barcelona, Spain
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An effect of drift is investigated on the segregation pattern in diffusion-limited aggregation (DLA) with two components (A and B species). The sticking probability P_{AB} $(=P_{BA})$ between the different species is introduced into the DLA model with drift, where the sticking probability P_{AA} $(=P_{BB})$ between the same species equals 1. By using computer simulation it is found that the drift has an important effect on not only the morphology but also the segregation pattern. Under the drift and the small sticking probability, a characteristic pattern appears where elongated clusters of A species and of B species are periodically dispersed. The period decreases with increasing drift. The periodic structure of the deposits is characterized by an autocorrelation function. The shape of the cluster consisting of only A species (or B species) shows a vertically elongated filamentlike structure. Each cluster becomes vertically longer with decreasing sticking probability P_{AB}. The segregation pattern is distinctly different from that with no drift and a small sticking probability P_{AA}. The effect of the concentration on the segregation pattern is also shown.

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I. INTRODUCTION

Recently there has been increasing interest in a variety of aggregation and deposition models such as diffusion-limited aggregation (DLA) and ballistic deposition [1–14]. The ballistic deposition model provides a basis for understanding deposition processes used to prepare a wide variety of thin-film devices. The DLA model presents a prototype of the pattern formation of diffusive systems including electrochemical deposition, crystal growth, viscous fingering, dielectric breakdown, chemical dissolution, and bacterial colonies. The DLA model is consistent with Laplacian growth. The DLA model with drift is interpolated between the DLA and ballistic models. A variety of computer simulations have been carried out to investigate the relationships between the cluster geometry and growth mechanisms. The structure of the aggregates strongly depends on the dynamics of the growth process. Also, various experiments have been performed to determine the morphological evolution under different experimental situations. Some distinct morphologies such as DLA fractals, dense patterns, and needle structures have been found by computational and experimental methods [15–22]. The morphological changes have also been analyzed by the real-space renormalization-group method [23–26].

Some computer simulations have shown that the drift has an important effect upon the morphology in DLA. With introduction of the attractive drift in DLA, the morphology crosses over from the DLA fractal at small length scales to the dense structure at large length scales. Up to now, most of the studies on pattern formation phenomena in this context refer to a single-component DLA. However, very few investigations for the DLA with two components have been performed. It will be interesting to study the morphology and the segregation in the DLA with two components. The two-component DLA with drift corresponds to such physical processes as the electrochemical deposition with two components under high applied voltages.

In a previous paper [27], we studied the morphological change in the two-component DLA by using a computer simulation. We introduced the sticking probability P_{AB} between the different species into the original DLA model. We found that various patterns of the composite deposits are produced by varying the sticking probabilities P_{AB} $(=P_{BA})$ and P_{AA} $(=P_{BB})$ where P_{AA} $(=P_{BB})$ is the sticking probability between the same species. With both sufficiently small sticking probabilities P_{AB} and P_{AA}, the overall shape of the deposit approaches that of a dense pattern and the segregation patterns of the composite deposits show a vertical laminar structure. However, it is an open question as to whether or not the drift has an effect on the segregation pattern of the composite deposit.

In this paper, we study the effect of the drift on the segregation pattern in the two-component DLA by using a computer simulation. We introduce the sticking probability P_{AB} between the different species into the DLA model with drift. Here, the drift is applied to mobile particles. We restrict ourselves to the case where the sticking probability P_{AA} $(=P_{BB})$ between the same species equals 1. The sticking probability refers to the affinity of each particle for sticking on each of the two components of the aggregate. We find that the drift has an important effect on not only the morphology but also the segregation pattern. We show that a characteristic pattern with periodically alternating structures of A cluster and B cluster appears under the drift and the small sticking probability. Also the shape of the cluster consisting of only A species (or B species) shows a vertically elongated filamentlike structure. We find that the segregation pattern obtained here is distinctly different from that with no drift and a small sticking probability P_{AA} (obtained in a previous paper). The effect of the concentration on the segregation pattern is also shown.

The organization of the paper is as follows. In Sec. II we present the model. In Sec. III we give the simulation algorithm and the results of our simulations. Finally, Sec. IV contains a brief summary.

II. MODEL

We present the two-component DLA model with drift. We consider the deposition process on a plate. We assume that A and B species diffuse independently under an attractive drift. The attractive drift works on the diffusive particles vertically to the plate. The concentrations C_A and C_B of diffusive components with the attractive drift satisfy respectively the distinct convective-diffusion equations under the quasistationary approximation

$$u\frac{\partial C_A}{\partial y}+D\nabla^2 C_A=0 , \tag{1a}$$

$$u\frac{\partial C_B}{\partial y}+D\nabla^2 C_B=0 , \tag{1b}$$

where u indicates the attractive drift toward the plate, D is the diffusion constant, the x axis is taken along the plate, and the y axis is taken as the vertical direction outward from the plate.

The boundary conditions far from the plate correspond to constant concentrations C_A and C_B. We turn now to the consideration of the boundary conditions on the surface of the deposit. We define the sticking probabilities P_{AA}, P_{BB}, P_{AB}, and P_{BA}. P_{AA} (P_{BB}) indicates the sticking probability at which the A (B) species sticks on the surface of the A (B) species when the A (B) species lands on the surface of the A (B) species. We restrict ourselves to the case of $P_{AA}=P_{BB}=1$. In this case, the particle sticks on the same species with probability 1. P_{AB} (P_{BA}) indicates the sticking probability at which the A (B) species sticks on the surface of the B (A) species when the A (B) species lands on the surface of the B (A) species. We restrict ourselves to the case of $P_{AB}=P_{BA}$. The boundary conditions are given by

$$(1-P)\frac{\partial C_A}{\partial n}-PC_A=0 , \tag{2a}$$

where $P=1$ if the A species lands on the surface consisting of A species, and $P=P_{AB}$ if the A species lands on the surface consisting of B species,

$$(1-P)\frac{\partial C_B}{\partial n}-PC_B=0 , \tag{2b}$$

where

$$P=\begin{cases}1 & \text{if the } B \text{ species lands on the surface consisting of } B \text{ species,}\\ P_{BA} & \text{if the } B \text{ species lands on the surface consisting of } A \text{ species.}\end{cases}$$

Here, $\partial C/\partial n$ is the derivative normal to the interface. By introducing the sticking probability P_{AB} ($=P_{BA}$) into the DLA model, one can take into account the mixing effect of the two components on the DLA structure. We analyze segregation patterns under the condition $P_{AB}<1$, assumed throughout the paper. The obvious physical meaning behind this condition is that the connection between the same species is easier than the connection between the different species, as a result, for instance, of a different electrodeposition mechanism of a metal on different substrates. In the following section, we consider the simulation procedure of the two convective-diffusion Eqs. (1a) and (1b) with the boundary conditions (2a) and (2b).

III. SIMULATION AND RESULT

We consider the simulation of the aggregation process satisfying Eqs. (1a) and (1b) with the boundary conditions (2a) and (2b). The two kinds of convective-diffusing particles can be simulated by using two different biased random walkers. The simulation of the two-component drift-diffusion-limited aggregation with the boundary conditions (2a) and (2b) is carried out with the use of a simple square lattice. We consider a subset of the square lattice enclosed by a square with 200×200 (units). We start out with an occupied plate on the bottom of the square. The lateral boundary is periodic. The A particle or the B particle is introduced one at a time at a randomly chosen point on the upper boundary. The A particle is introduced with the probability $p=C_A/(C_A+C_B)$ and the B particle with the probability $1-p$. Each particle performs a biased random walk resulting from the attractive drift. The particle continues to move until it either reaches a point adjacent to a site already occupied by a particle or until it reaches the upper boundary. When the particle reaches a point adjacent to a site already occupied by a particle and if the already occupied site is of the same kind of particle, it sticks on the aggregate with probability 1. If the already occupied site is of a different kind of particle, it sticks on the aggregate with the probability P_{AB} ($=P_{BA}$). Otherwise, the particle is reflected at the aggregate with the probability $1-P_{AB}$ and continues to move. When the particle reaches the upper boundary, the random walker is annihilated. We repeat the above procedure. The deposits are grown until the height reaches 150 units. In the following, we study the two cases: (i) $0 < P_{AB} < 1$, variable u/D, and $p=0.5$, and (ii) $P_{AB}=0.01$, $u/D=0.1$, and variable p.

A. The case of $0 < P_{AB} < 1$, variable u/D, and $p=0.5$

First, we investigate the effect of the drift on the morphology and segregation. We set the concentration fraction as $p=0.5$ (equal concentration). Figures 1(a)–1(c) show, respectively, the simulation results for $u/D=0.01$, 0.1, and 0.3 under the condition $P_{AB}=0.1$. The upper, middle, and bottom patterns in each figure indicate, respectively, the deposits consisting of A and B species, only A species within the composite deposit, and only B species within the composite deposit. The simulation result is obtained by using the procedures outlined above. With increasing drift u/D, the morphology of the deposit becomes more dense. Figures 2(a)–2(c) show, respectively, the simulation results for $u/D=0.01$, 0.1, and 0.3 under $P_{AB}=0.01$. Under the small sticking probability P_{AB}, the segregation occurs and the large clusters consisting of A species or B species appear. With increasing drift u/D, the morphology becomes not only dense, but also the segregation pattern changes distinctly. Each cluster becomes a vertically elongated structure with increasing drift u/D. With increasing drift u/D, each cluster becomes a less ramified structure. The elongated clusters of A species and of B species are periodically dispersed. The period decreases with increasing drift. Figures 3(a)–3(c) show, respectively, the simulation results for $u/D=0.01$, 0.1, and 0.3 under $P_{AB}=0.001$. With the very small sticking probability, more elongated clusters appear. With increasing drift u/D, a vertically elongated filamentlike structure appears. With decreasing sticking probability P_{AB}, the filamentlike clusters become more elongated under the drift.

Here we compare our simulation result with a previous result [27]. In a previous paper, we performed computer simulation for the morphology and segregation in the two-component DLA without drift. We found that the characteristic patterns were produced with varying the sticking probabilities P_{AB} $(=P_{BA})$ and P_{AA} $(=P_{BB})$. Figure 4 shows the simulation result for $P_{AB}=0.001$, $P_{AA}=0.1$, $u/D=0$, and $p=0.5$. This can be compared with Fig. 3(b) ($P_{AB}=0.001$, $P_{AA}=1$, $u/D=0.1$, and $p=0.5$). The morphology in Fig. 4 is consistent with that of Fig. 3(b). However, the segregation pattern in Fig. 4 is different from that of Fig. 3(b). The cluster is elongated by the drift. The cluster becomes thicker by small sticking probability P_{AA}. Figure 5 shows the simulation result for $P_{AB}=0.001$, $P_{AA}=0.01$, $u/D=0$, and $p=0.5$. This can be compared with Fig. 3(c) ($P_{AB}=0.001$, $P_{AA}=1$, $u/D=0.3$, and $p=0.5$). The

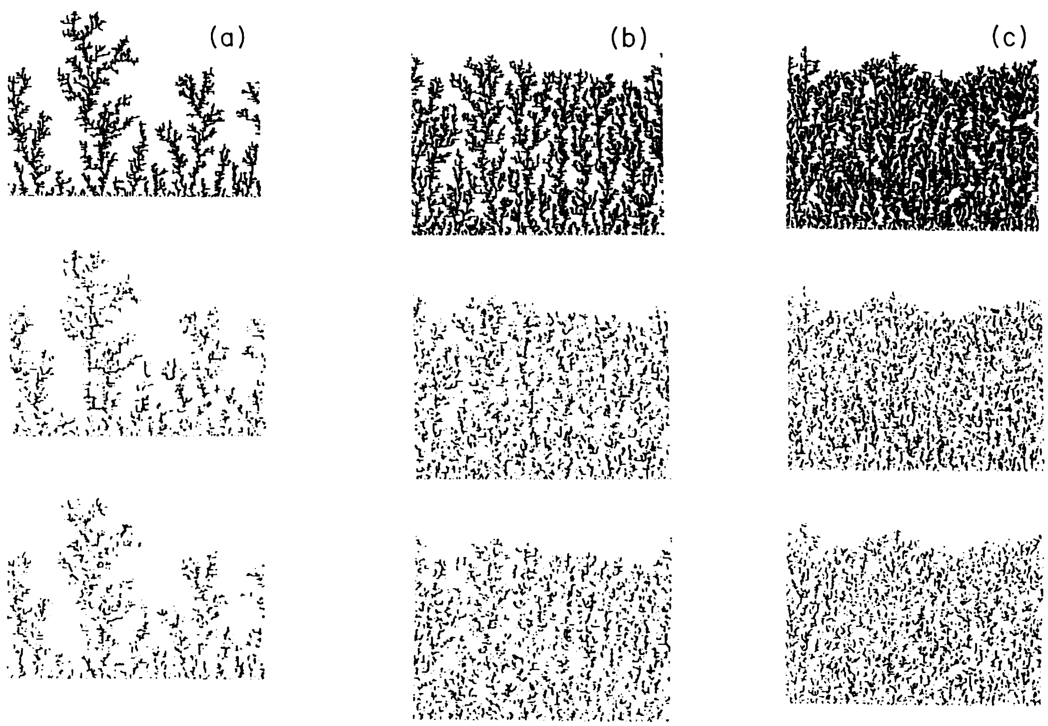

FIG. 1. Typical patterns of the composite deposits grown by varying the strength of drift u/D for fixed sticking probability $P_{AB}=0.1$ and composition ratio $p=0.5$. The upper, middle, and bottom patterns in this and Figs. 2–5,7 indicate, respectively, the composite deposits consisting of A and B species, only A species within the deposit, and only B species within the deposit. (a) $u/D=0.01$. (b) $u/D=0.1$. (c) $u/D=0.3$.

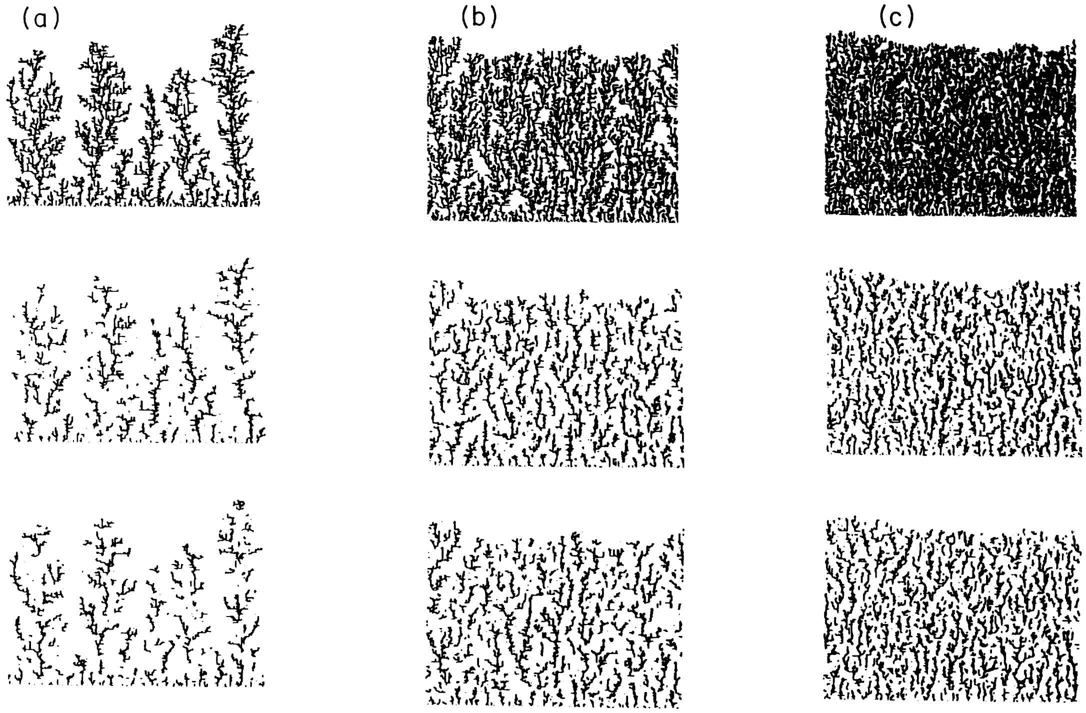

FIG. 2. Typical patterns of the composite deposits grown by varying the strength of drift u/D for $P_{AB}=0.01$ and $p=0.5$. (a) $u/D=0.01$. (b) $u/D=0.1$ (c) $u/D=0.3$.

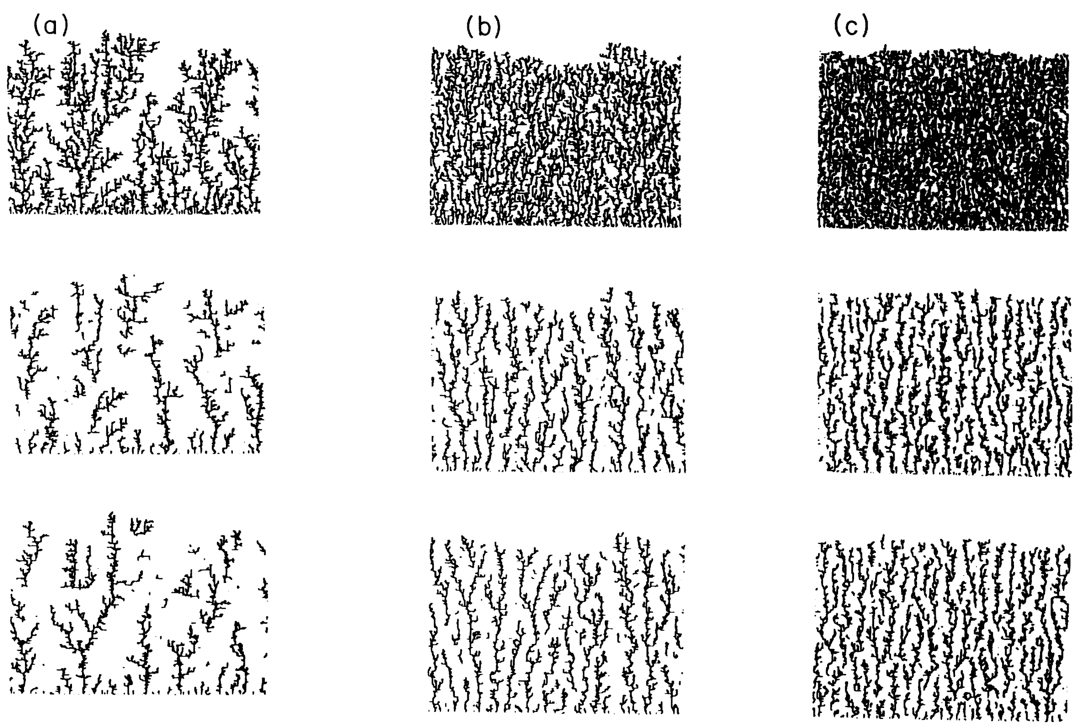

FIG. 3. Typical patterns of the composite deposits grown by varying the strength of drift u/D for $P_{AB}=0.001$ and $p=0.5$. (a) $u/D=0.01$. (b) $u/D=0.1$. (c) $u/D=0.3$.

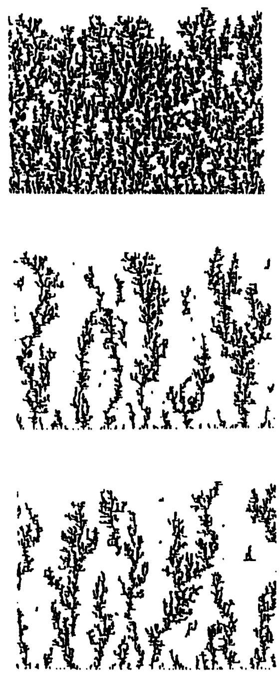

FIG. 4. Typical pattern of the composite deposit without drift for $P_{AB}=0.001$, $P_{AA}=0.1$, $u/D=0$, and $p=0.5$. This can be compared with Fig. 3(b).

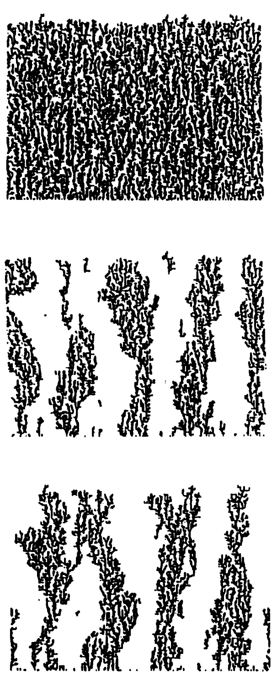

FIG. 5. Typical pattern of the composite deposit without drift for $P_{AB}=0.001$, $P_{AA}=0.01$, $u/D=0$, and $p=0.5$. This can be compared with Fig. 3(c).

morphology in Fig. 5 is consistent with that of Fig. 3(c). However, the segregation pattern in Fig. 5 is different from that of Fig. 3(c). The segregation pattern in Fig. 5 shows the striped structure. The segregation pattern in Fig. 3(c) shows the filamentlike structure.

We calculate the autocorrelation function to characterize the periodic structure of the segregation pattern in the two-component DLA with drift. We define the autocorrelation function

$$\xi(x)=(1/N)\sum_{x'}\rho(x')\rho(x+x') . \tag{3}$$

Here, if the site x is occupied by A species, $\rho(x)=1$. Otherwise, $\rho(x)=0$. The summation ranges over all the sites on the horizontal line. N indicates the total number of particles on the horizontal line. We calculate the autocorrelation function at the height $h=75$. The autocorrelation functions show the periodic structure. The distance between peaks represents the period. Figure 6 shows the period T plotted against drift u/D for $P_{AB}=0.01$ and $p=0.5$. With increasing drift, the period between A clusters decreases. The period approaches the limit value $T\approx5$.

B. The case of $P_{AB}=0.01$, $u/D=0.1$, and variable p

Second, we study the effect of the concentration on the morphology and the segregation. Under the condition of $P_{AB}=0.01$, and $u/D=0.1$, we vary the concentration fraction p. Figures 7(a)–7(c) show, respectively, the patterns for $p=0.3$, 0.5, and 0.7. The morphology becomes more dense with increasing concentration fraction p (<0.5). At $p=0.5$, the morphology becomes most dense. Then, the morphology becomes less dense with increasing p (>0.5). With increasing concentration fractions, clustering of A species occurs. Above $p=0.5$, the clusters of A species are connected between the bottom and the top. Near $p=0.5$, a percolation transition occurs. The A

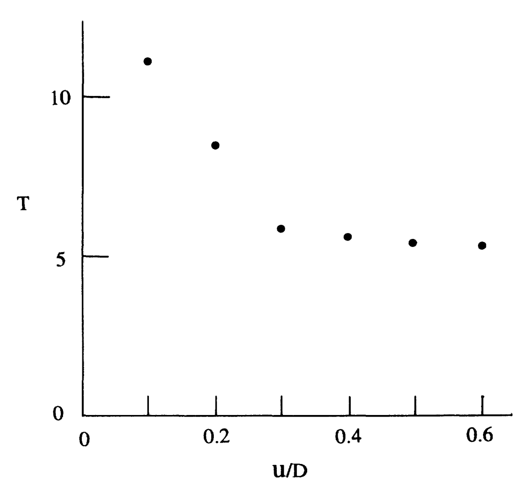

FIG. 6. The period T between A clusters plotted against drift u/D.

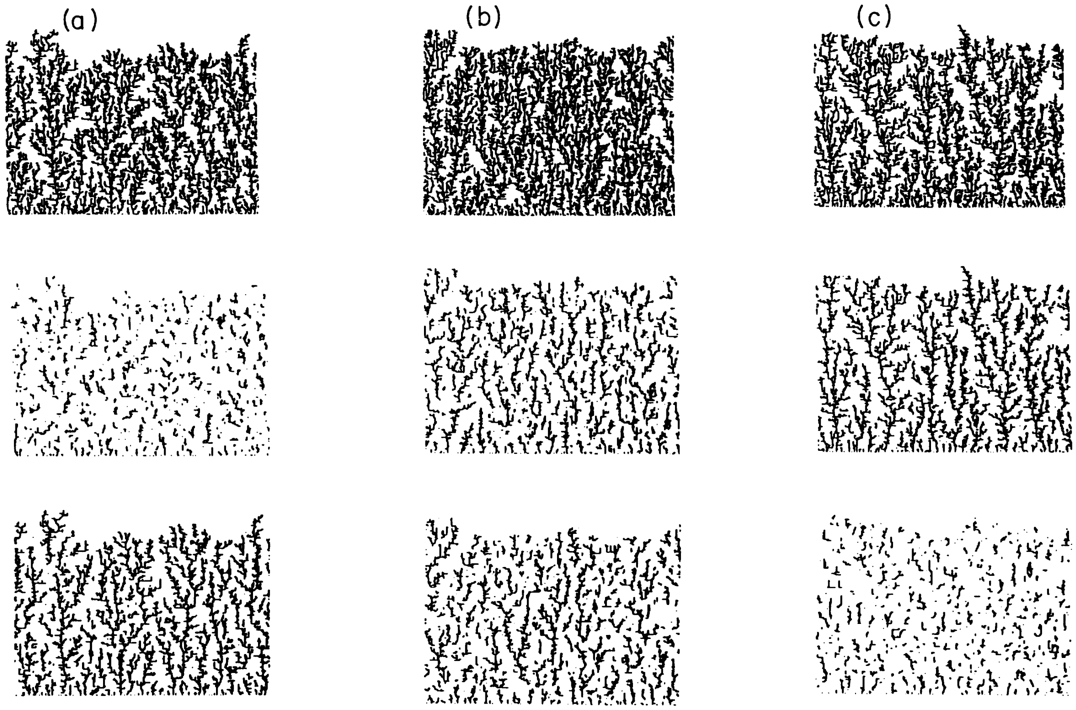

FIG. 7. Typical patterns of the composite deposits grown by varying the concentration fraction p for $P_{AB}=0.01$ and $u/D=0.1$. (a) $p=0.3$. (b) $p=0.5$. (c) $p=0.7$.

cluster percolates from the bottom to the top above $p=0.5$. This result is similar to the original percolation phenomena [28]. We find that the concentration fraction p has an important effect on the segregation pattern.

IV. SUMMARY

We investigate the effect of the drift on the segregation pattern in the two-component DLA. We introduce the drift into the two-component DLA model. By using computer simulation, we find that the drift has an important effect on not only the morphology, but also the segregation pattern. Under the drift and the small sticking probability P_{AB}, we show that a characteristic pattern with periodically alternating elongated clusters appears. We calculate the autocorrelation function to characterize the periodic segregation pattern. We also show that the concentration p has an important effect on the segregation pattern.

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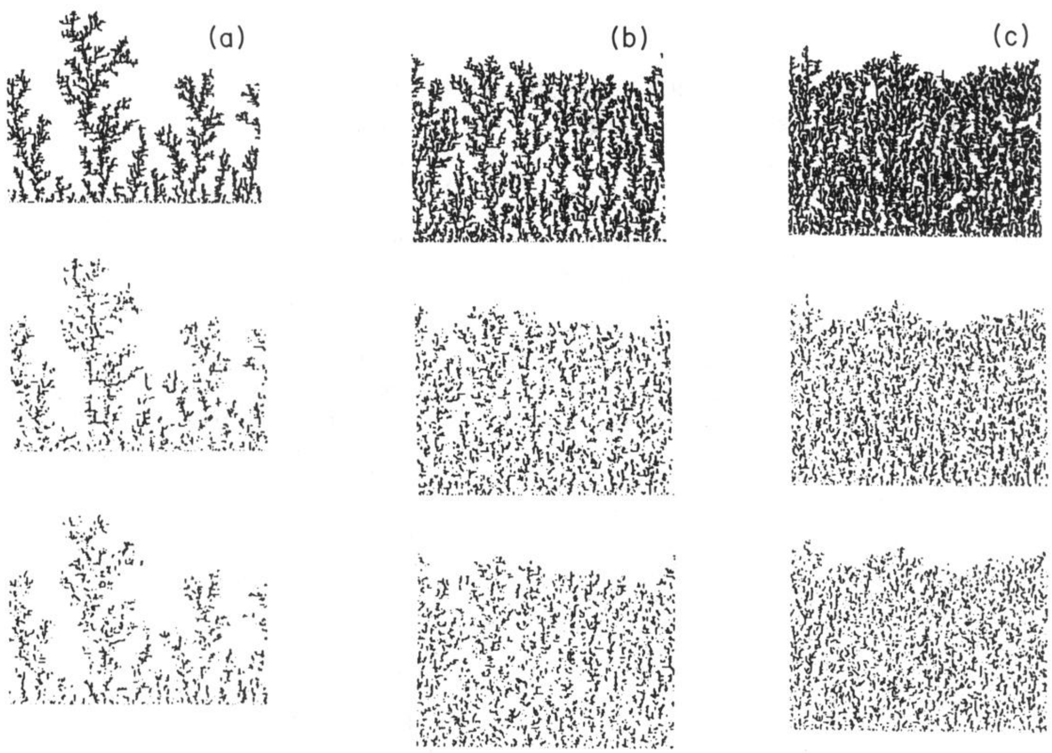

FIG. 1. Typical patterns of the composite deposits grown by varying the strength of drift u/D for fixed sticking probability $P_{AB}=0.1$ and composition ratio $p=0.5$. The upper, middle, and bottom patterns in this and Figs. 2–5,7 indicate, respectively, the composite deposits consisting of A and B species, only A species within the deposit, and only B species within the deposit. (a) $u/D=0.01$. (b) $u/D=0.1$. (c) $u/D=0.3$.

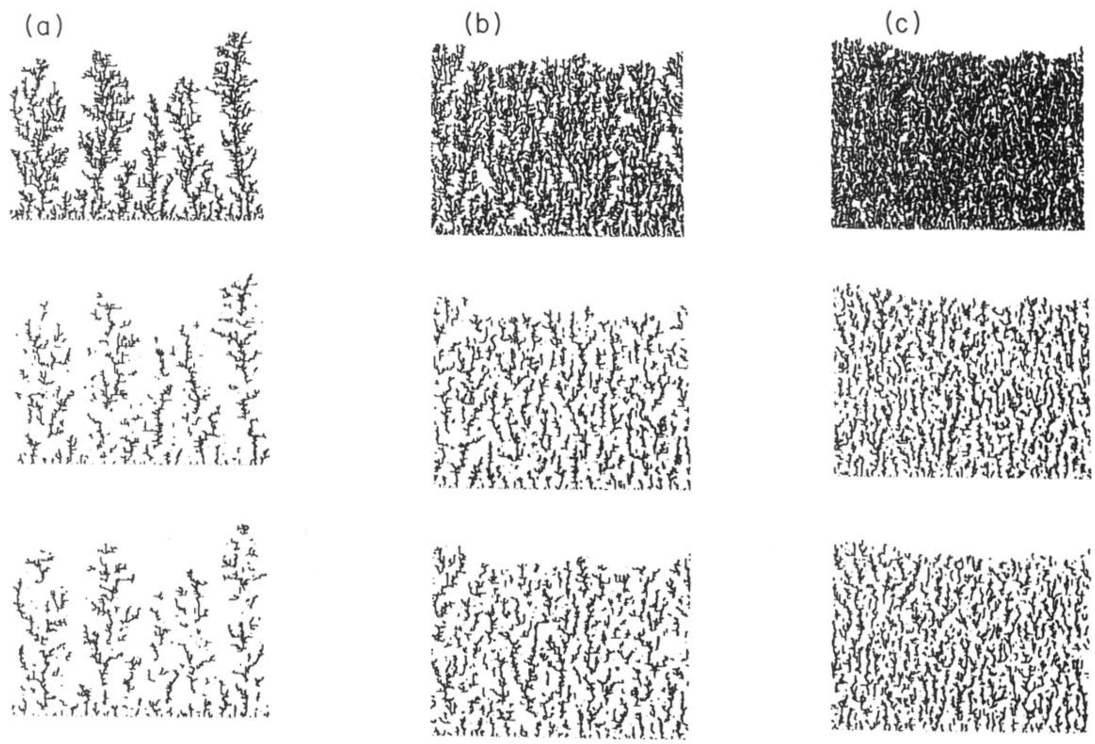

FIG. 2. Typical patterns of the composite deposits grown by varying the strength of drift u/D for $P_{AB}=0.01$ and $p=0.5$. (a) $u/D=0.01$. (b) $u/D=0.1$ (c) $u/D=0.3$.

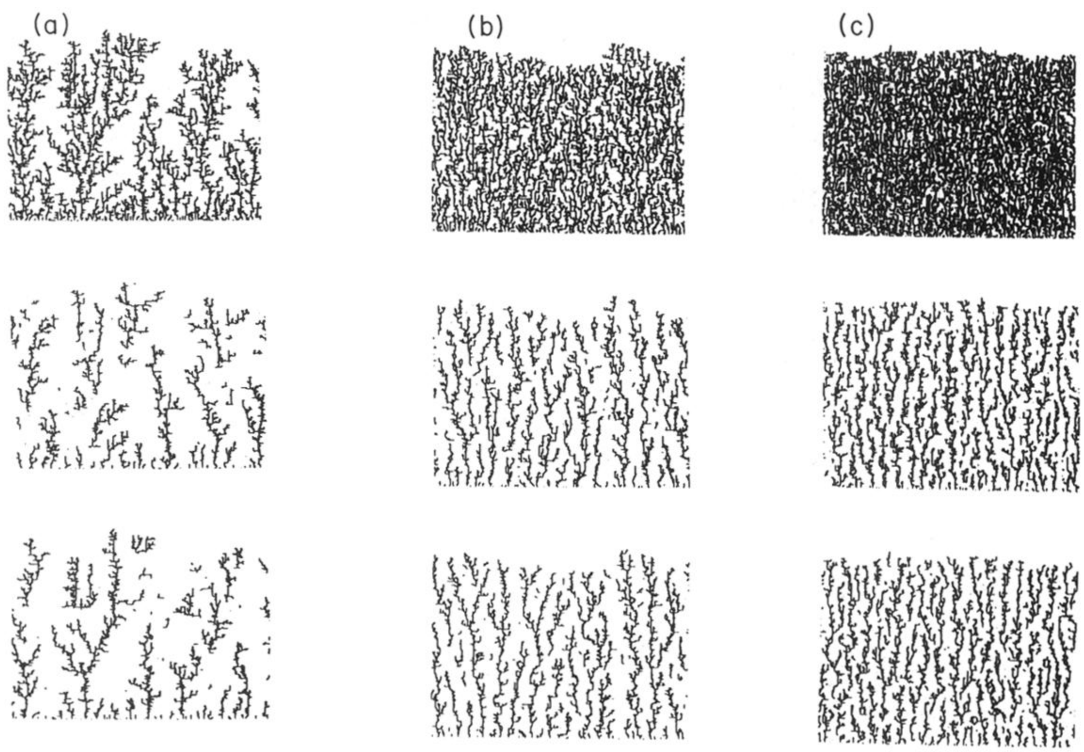

FIG. 3. Typical patterns of the composite deposits grown by varying the strength of drift u/D for $P_{AB}=0.001$ and $p=0.5$. (a) $u/D=0.01$. (b) $u/D=0.1$. (c) $u/D=0.3$.

FIG. 4. Typical pattern of the composite deposit without drift for $P_{AB}=0.001$, $P_{AA}=0.1$, $u/D=0$, and $p=0.5$. This can be compared with Fig. 3(b).

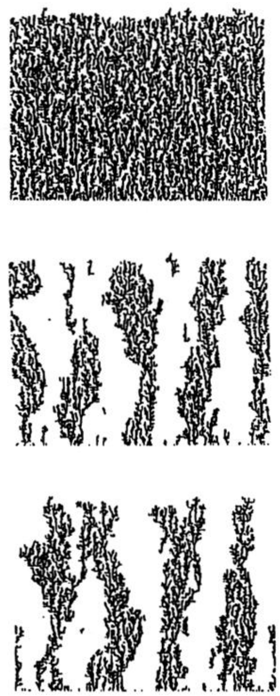

FIG. 5. Typical pattern of the composite deposit without drift for $P_{AB}=0.001$, $P_{AA}=0.01$, $u/D=0$, and $p=0.5$. This can be compared with Fig. 3(c).

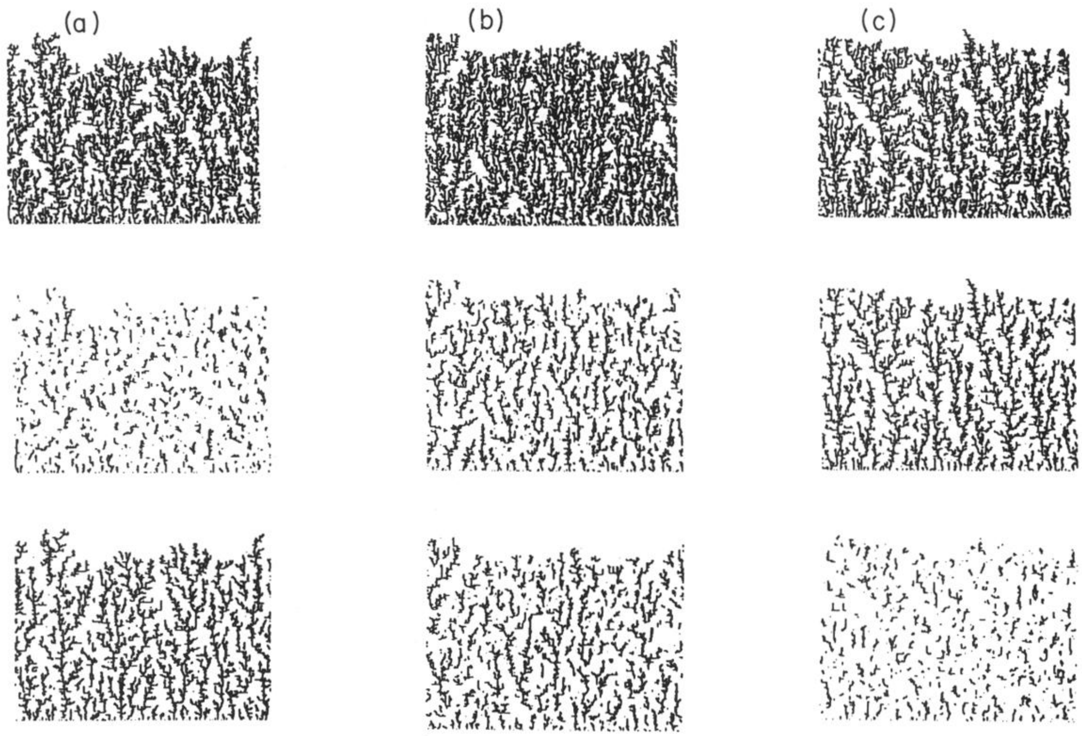

FIG. 7. Typical patterns of the composite deposits grown by varying the concentration fraction p for $P_{AB}=0.01$ and $u/D=0.1$. (a) $p=0.3$. (b) $p=0.5$. (c) $p=0.7$.