Kinetic growth of randomlike and ballisticlike deposition models

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The pattern structure and the scaling behavior of the surface width for two deposition models of two kinds of particles, particle A with a probability 1-P and particle C with a probability P, depositing on a (1+1)-dimensional substrate are studied. For model I, a randomlike deposition model, the pattern has a compact structure, and the surface width growth only depends on the time, $W \sim t^{1/2}$ for the early stage and $W \sim t^{\beta(P)}$ for the intermediate time where β is a function of P, as well as $W \sim P^{-\gamma}$ for the later time. For model II, a ballisticlike deposition model, the pattern and scaling behavior are similar to the ballistic deposition. The scaling of the surface width is $W \sim t^{\beta(P)}$ for the early stage of growth and $W \sim L^{\alpha}$ for the later stage. The exponent β is a function of P, while α is independent of P.

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I. INTRODUCTION

Recently, there has been considerable interest in the study of the morphology of growing surfaces or interfaces, not only because of its potential technological importance, but also due to its manifestation of interesting nonequilibrium statistical physics at fundamental levels [1]. Most of these studies contain rough surfaces and stochastically growing interfaces in the context of ballistic deposition [2], the Eden model [3,4], and the solid-onsolid model [5,6], as well as the molecular-beam deposition [7,8] and the continuum stochastic equation of Kardar, Parisi, and Zhang (KPZ) [9].

A novel feature of this phenomenon is the existence of scaling [10], i.e., if we start at t = 0 from a flat surface of length L, we have

$$W(L,t) = L^{\alpha} f(t/L^{z}) , \qquad (1)$$

where W(L,t) is the rms roughness of the surface, or the surface width

$$W^{2}(L,t) = \frac{1}{L^{d-1}} \sum_{r} [h(r,t) - \overline{h(t)}]^{2}.$$
 (2)

Here h(r,t) is the height of the surface at position r and time t, h(t) is the average height at time t, and d'=d-1is the substrate dimension in d-dimensional space. The roughness exponent α characterizes the self-affine fractal nature of the surface represented by the scaling $W \sim L^{\alpha}$, in the long-time limit. At the early stage of growth $t \ll L^z$ the scaling function $f(t/L^z)$ is such that $W \sim t^{\beta}$, where $\beta = \alpha/z$ and z is the dynamic exponent.

A phenomenological equation, which applies to a large class of surface growth models, is the KPZ equation [9]

$$\frac{\partial h}{\partial t} = v \nabla^2 h + (\lambda/2)(\nabla h)^2 + \eta(r, t) , \qquad (3)$$

where the noise $\eta(r,t)$ satisfies $\langle \eta(r,t)\eta(r',t')\rangle$ $=2D\delta(r-r')\delta(t-t')$. It is a nonlinear equation for the time dependence of the interface height h(r,t) in a ddimensional system, above a (d-1)-dimensional plane. The KPZ equation has been quite successful in describing a wide variety of growth models, including ballistic aggregation, the Eden model, and vapor deposition [1].

The diffusion-limited-aggregation model produces a self-similar fractal structure [11]. The Eden model and the ballistic-deposition model give rough surfaces that are self-affine but not self-similar. Various models that are used for the study of surface phenomena only concern the growing of one kind of particle [1]. However, in the growing of real materials one may take into consideration that different particles are deposited on these structures (i.e., alloys or impurities). Thus, in the growing system, there may exist different interactions for different particles. The growing mechanism will also be changed.

In this paper we describe the kinetic growth of the deposition of two kinds of particles A and C (particle A with probability 1-P and particle C with probability P) on a d-dimensional substrate, using two different models: (i) randomlike deposition and (ii) ballisticlike deposition. The organization of this paper is as follows. In Sec. II, we present the models and the results of the aggregation patterns. In Sec. III, the dynamical scaling behavior of the surface width Eq. (1) is studied. In the last section, we give the summary.

II. MODELS AND AGGREGATION PATTERNS

We consider the deposition of two different kinds of particles, particle A (the active particle) and particle C (the nonactive particle) onto a d-dimensional substrate. In the initial configuration all sites on the substrate are occupied by particle A. The particles are allowed to fall straight down randomly, one at a time, onto a growing surface and stick where they land according to the models described below. In both models, first a site is chosen randomly, and then with probability 1-P (or P) a particle A (or particle C) is deposited on the surface of the aggregation depending on the following conditions.

Model I. The deposition occurs when the particle on the top of the chosen site is particle A, or if the particle on the top of the chosen site is particle C and one of the nearest neighbors (one unit higher than the top of the chosen site) is particle A.

Model II. The deposition occurs once the dropping particle first encounters a particle A wherever it is on the top or the tops of the two nearest-neighbor columns of the chosen site. For instance, if the dropping particle falls down along column i, and it first meets a particle A, which is on the top of the column i+1 (no matter what kind of particle is on the top of column i), this dropping particle will stick to this particle A and the falling stops. Obviously, if the dropping particle first meets a particle A which is just on the top of column i, it stops and deposits there. It is clear that the difference between model II and model I is whether sticking to the side of a column is allowed or not.

Obviously, model I is a randomlike deposition model. For P = 0, the deposition of model I is just the same as the random model [10], which is a trivial surface growth model in which a particle simply falls until it reaches the top of a column. Since there are no correlations between the columns, these grow independently; however, the surface is rough. When $P\neq 0$ once a particle C is deposited on a column, its growth will depend on the nearest neighbors. This introduces a correlation between the different columns. For a larger P, the growth of the aggregation may reach a saturation state earlier than that of the case of smaller P. However, the situation is different for model II since this represents a ballisticlike deposition which is a nontrivial model: there is a strong correlation between different columns. When P=0, model II is the usual ballistic model [2]. Similarly, when $P \neq 0$, the deposition process will be affected by the existence of particle C; the aggregation may stop with larger P. But the "lifetime" of the system is much longer than that of model I, and also the scaling behavior gives rise to some interesting results (discussed in the following section).

These models may represent the chemical reactions which take place in the surface of the growth of materials. For example, we model the following reaction process:

$$A + B = C . (4)$$

Particle A and particle B are active, and once particle A is touched by a particle B the combination produces a reactant C which is no longer active. The particle A is chosen with a probability 1-P, and the particle B with P, i.e., the reactant C is produced with the probability P. Thus, in these systems, some of the surface sites continue to react while some sites do not. The initial flat substrate placed with particle A is for the reactions.

These models can also represent a growing interface of a material with a low concentration of impurities. Our models mimic the role of the impurity atoms as follows. An impurity atom (particle C) is introduced with a probability P while it has a less active bond for other atoms (particle A).

In the present paper, we report on the simulation of a (1+1)-dimensional case. The substrate is a strip with the

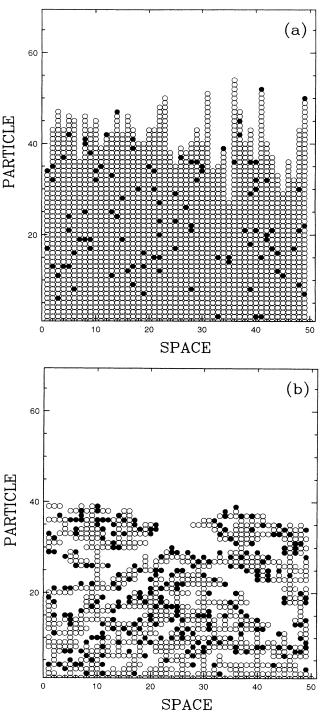


FIG. 1. Structure of the deposition (half part of the system L=100). The open circles represent particle A and the solid circles represent particle C. (a) Model I with P=0.05; (b) model II with P=0.2.

width L (in the X direction). The aggregation is in the Y direction. At the beginning, all sites are occupied by particle A for $Y \le 0$. A periodic boundary condition is used in the L direction (in the X direction). The typical size of system L used in our simulation is L = 100. Some runs on smaller and larger L have also been done.

In Fig. 1(a), we show one example of the aggregation for model I with P = 0.05. From this figure we see that the surface is rough and the structure of the aggregate is compact. Due to the correlation between the nearest neighbors, particle C's (or the impurity atoms) are surrounded by particle A's. We can expect that if the probability P is very large the deposition will stop, i.e., the aggregation will not grow more when all the surface sites are covered by particle C.

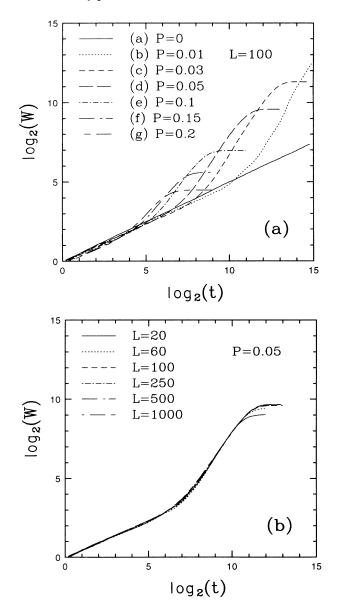


FIG. 2. Log-log plots of the surface width W(t) against t, the numbers of the deposited particles. (a) With different probability P and same system size L=100; (b) with the same probability P=0.05 and different system sizes.

TABLE I. Relationship between the probability P and the exponent β and the saturation value of the surface width for model I.

P	β	$\log_2 W \ (t = \infty)$
0	$\frac{1}{2}$	∞
0.01	1.80	
0.03	1.66	11.25
0.05	1.54	9.6
0.1	1.36	7.0
0.15	1.22	5.6
0.2	1.16	4.5

In Fig. 1(b), we have showed an example of the pattern of the ballisticlike aggregation model II with $P\!=\!0.2$. Although there are some vacancies or holes in the bulk of the ballistic deposition, it is not a self-similar fractal because the density of the aggregate is finite. However, the surface of the deposit is a self-affine fractal and its evolution can be described by the dynamical scaling approach, which will be discussed in the following section.

III. DYNAMICAL SCALING BEHAVIOR

Figure 2(a) shows a plot of the surface width W with time for different deposition probabilities for model I. The system size is L=100 and the statistic average is found by averaging over 50 runs. Curve (a) shows the case of the random deposition of only one kind of particle (particle A), i.e., with P=0 for particle C. As we have seen in Fig. 1(a), since there are no correlations between the columns, the height of the columns follows a Poisson distribution [10]. The width of the surface is proportional to the square root of the time t, $W \sim t^{1/2}$, i.e., $\beta = \frac{1}{2}$, independent of the dimension [10]. There is no saturation width, that is, no steady state. While $P \neq 0$, the scaling behavior is changed. From curves (b)-(g) showed in

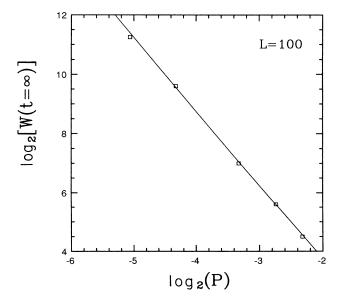


FIG. 3. Log-log plot of the saturation value $W(t = \infty)$ against the probability P.

Fig. 2(a) for different deposition probabilities of the particle C there exists a steady state. The growth of the aggregation is divided into two stages. At the early time, the width grows with a power of time $W \sim t^{1/2}$, the same as the random deposition. Then just before saturation, the width grows with a power of time $W \sim t^{\beta}$. Here β is a function of P, $\beta = \beta(P)$. In Table I, we present the relationship between β and P, as well as the saturated values of the surface widths. We see that β increases with P, however, the saturated values of the surface width W decreases.

Figure 2(b) shows a plot of the surface width of the deposition for the randomlike growth (model I) as a function of time for different sizes of the system and for the same probability P = 0.05. From this figure, we see that

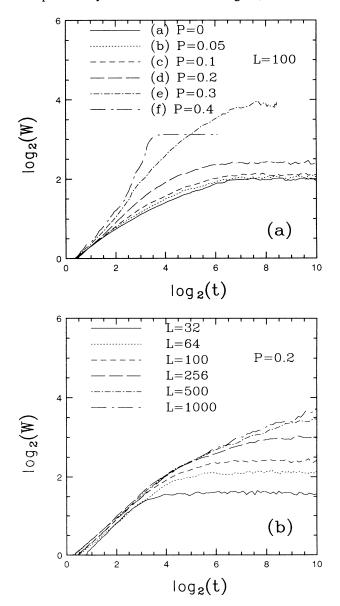


FIG. 4. Log-log plots of the surface width W(t) against t, the number of deposited particles per site. (a) With different probability P and same system size L=100; (b) with different system size L and same probability P=0.2.

the surface width is independent of the system size and the curves collapse onto one, except for L=20 and 60 because of the finite-size effect. We have done the same simulation for different values of P and we got the same conclusion. Thus, the scaling behavior is different from Eq. (1) of our model I. In our opinion, this independence of the system size of the surface width is due to the weak correlation between the columns. Instead of this independence of the saturated surface width with the system size, the surface width can be scaled with the probability P:

$$W(t = \infty) \sim P^{-\gamma} = P^{-5/2}$$
 (5)

In Fig. 3, we have plotted the saturated values of the surface width $W(t=\infty)$ against the probability P for L=100. One can see that the slope of the plot is $\gamma=\frac{5}{2}$. Since $W(t=\infty)$ is independent of the system size, the exponent γ has the same value, for different system sizes. We have done two runs for L=100 and 500, respectively, and the points are coincident in Fig. 3.

Meanwhile, the case is very different for model II and the scaling behavior similar to Eq. (1). In Fig. 4(a), we show the surface width for different values of the probability but with the same system size fixed with L = 100. For each curve the statistical average is obtained by averaged over 400 runs, except for L = 1000, which is averaged only over 100 runs. Curve (a) shows the case of ballistic deposition with only one kind of particle (particle A). The best numerical estimates indicate that for ballistic deposition in d=2, $\beta=\frac{1}{3}$, and $\alpha=\frac{1}{2}$ [12]. Our results recover these exponents very well. However when $P\neq 0$, the exponent β is different. From curves (b)-(f)plotted in Fig. 4(a) we can see that the surface width evolves according to $W \sim t^{\beta(P)}$ (here we have put β as a function of P). After some time, the surface width saturates. The exponent β and the saturated values of the surface widths $W(t = \infty)$ with respect to P are present in Table II. From Table II, we see that as the probability P increases, the exponent β also increases which means the process of deposition has slowed down. For P = 0.4, the probability of the deposition of particle C is so large that the deposition is stopped before the surface width reaches the saturated value. Thus we leave $W(t = \infty)$ empty in Table II.

In Fig. 4(b), we plot the surface width W against time for different system sizes and with the probability P=0.2. From this figure one get the exponent α . Within the error of the calculation, we got $\alpha=\frac{1}{2}$, the value for the case of the usual ballistic model. We have

TABLE II. Relationship between the probability P and the exponents β for model II.

P	β	
0	$\frac{1}{3}$	
0.05	0.38	
0.1	0.44	
0.2	0.57	
0.3	0.70	
0.4	0.75	

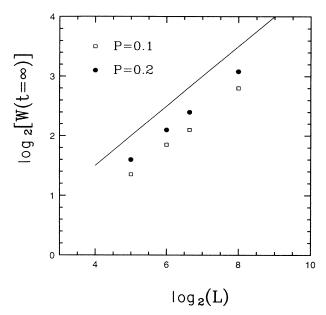


FIG. 5. Log-log plot of saturation value $W(t = \infty)$ against the system size L for the probability P = 0.1 and 0.2.

also checked this result for other values of the probability, for example, P = 0.1. The results are plotted in Fig. 5.

IV. SUMMARY

In this paper, we have studied the kinetic growth for the randomlike and ballisticlike models. After introducing both models we have presented the growing patterns, and then we have studied the dynamical scaling behavior. For the randomlike growth model, we found that due to the weak correlation of the aggregation, the pattern has a compact structure, and in the early time of the deposition the surface width can be scaled as $W \sim t^{1/2}$, while $W \sim t^{\beta(P)}$ for the intermediate time. Then follows a saturation which is independent of the system size, i.e., the exponent $\alpha=0$, but depends on the probability P, $W(t=\infty) \sim P^{-\gamma}$ with $\gamma=\frac{5}{2}$. For the ballisticlike model, model II, the pattern and scaling behavior is similar to the ballistic deposition. The scaling of the surface width can be described by $W \sim t^{\beta(P)}$, with the exponent β being a function of P, the probability, for the early stage of the deposition. The α exponent is independent of P and equals to the value of the usual ballistic deposition $\alpha=\frac{1}{2}$.

In Ref. [13], Keefer and Schaefer developed a variation of the Eden model to study the growth and structure of fractally rough silicate particle clusters by considering the details of the silicate chemical process. In their model the active bonds (n) and nonactive bonds (4-n) of each monomer are modeled by a random functional. Our models are different from theirs since we only consider the deposition process of two kinds of particles with different bonds, and in addition, we have not included the diffusion of particle C. We expect that considering this diffusion the scaling behavior of the kinetic process will change. The extension of such study to higher dimensions is currently under examination.

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