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Surface growth kinetics and morphological structural transition in a (2 + 1)-dimensional deposition model

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Abstract. A new ballistic-like surface growth model of two kinds of particle (A and C) depositing on a two-dimensional substrate is proposed. The scaling behaviour of the surface width W is obtained for different values of the deposition probability P of particle C and system sizes. As the probability P increases a transition of the morphological structure is found, which is defined by the exponent β varying with the probability P. The physical origin of the transition is discussed in terms of the diffusion of particles and the directed percolating processes.

1. Introduction

The growth of rough surfaces and interfaces has been a subject of considerable interest because of its technological importance, and its relevance for understanding nonequilibrium statistical physics at fundamental level [1, 2]. A dynamical scaling behaviour has been found by Family and Vicsek [3]. On defining the surface width $W(L,t)$ by

$$W^2(L,t) = \frac{1}{L^{d-1}} \sum_r \left[h(r,t) - \overline{h(t)} \right]^2 \tag{1}$$

where L is the system size, $h(r,t)$ is the height of the surface at position r and time t, and $\overline{h(t)}$ is the mean surface height, the scaling law is given by

$$W(L,t) = L^{\alpha} f(t/L^z). \tag{2}$$

The dynamical scaling behaviour is characterized by the roughness exponent α, and the dynamical exponent β, with $z = \alpha/\beta$. The scaling function $f(x)$ behaves as $f(x) = x^{\beta}$ for $x \ll 1$ and $f(x) = c$ for $x \gg 1$, with c being constant. This scaling behaviour has been studied in various systems and models, and has been argued to be universal [1, 2]. One successful theoretical approach is the Kardar–Parisi–Zhang (KPZ) approach [4], based on Edwards and Wilkinson's theory [5]. The KPZ equation is a nonlinear Langevin equation

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(x,t) \tag{3}$$

for the local growth of the profile $h(x,t)$ of a moving interface about a $(d-1)$-dimensional flat substrate [4]. Scaling arguments (power counting) as well as a one-loop renormalization-group (RG) calculation applied to equation (3) show that weak noise is relevant for

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$d < d_c = 2$, and irrelevant for $d > d_c$ [4, 6]. For spatial dimension $d = 2$ (substrate dimension $d' = d - 1$), the results for ballistic deposition, the Eden model, and the KPZ equation [4, 6, 7, 8] agree, giving $\alpha = 1/2$ and $\beta = 1/3$. However, for $d > 2$ there is still disagreement over the values of the exponents as well as the universality of the various surface growth models [9]. In addition, the RG analysis indicated the possibility of a nonequilibrium roughening transition from the weak-coupling to a strong-coupling regime for $d > d_c$. It has also been suggested that anomalous roughening behaviour may arise at the transition. Recently, some new understanding of the phase transitions for $3+1$ dimensions and above and weak–strong-coupling crossovers for $2+1$ dimensions and below of the KPZ equation have been achieved (see [10–12] and references therein). Some work on these and other growth models for various dimensions has been reported (see [10–15] and also the excellent review articles in [1, 2, 16] and references therein). Several typical examples are as follows. Amar and Family [13] used a generalization of the restricted solid-on-solid growth model of Kim and Kosterlitz [9]. On the other hand Yan, Kessler and Sander [14] introduced an *ad hoc* parameter P whose effect is to smooth the surface exactly as the Laplacian term does in the KPZ equation. Pellegrini and Jullien [15] made an interpolation between the nonrestructured and the completely restructured ballistic model, considering a random binary mixture of particles that slide or stick to the deposit upon contact. Tang, Nattermann and Forrest made a comparison between their hypercube-stacking model with deposition and evaporation of the particles and their renormalization-group treatment (see [10–12]). They all found that the system exhibits a phase transition as a function of a temperature-like parameter in $2 + 1$ or in higher dimensions. The phase transition is considered as a nonequilibrium analogue of the roughening transition. However, it is still important to know whether the observed roughening transition or the morphological structure transition will appear for more general surface growth cases by studying the discrete models with continuously tunable parameters which may be related to those in the KPZ equation. These may provide new insight into the dynamics of the surface growth for $d > 2$.

So far we know that the ballistic deposition model [3, 17, 18] and the Eden model [19–21], as well as some other surface growth models, give rough surfaces that are self-affine but not self-similar [1, 2]. Among them, a well-studied example is the ballistic deposition model. In this model, particles rain down vertically onto a $(d - 1)$-dimensional substrate and aggregate upon first contact. Such a model gives rise to a rather interesting structure; the surface is a self-affine fractal [1, 2] although the bulk is not compact, and has been extensively studied both on [17] and off [22] the lattice. Although the models described above have been proposed for studying the surface growth in $1 + 1$ and $2 + 1$ dimensions, as well as higher dimensions, all of them are only concerned with the growing of one kind of particle system [1, 2, 16]. Generally, in the growth of real materials one should take it into consideration that different kinds of particle are deposited on these structures, such as impurities in materials. Thus, in the growing system, there may exist different interactions for different particles and the growing mechanisms may also be different.

Following our previous study for the $(1 + 1)$-dimensional case [23, 24], here we report further results of a new surface growth model of two different kinds of particle, namely, the ballistic-like deposition model, in $2 + 1$ dimensions. We describe the kinetic growth of the deposition of two kinds of particle A and C (particle A with probability $1 - P$ and particle C with probability P) on the substrate. We use the probability P as a continuously tunable parameter to control the system. We study the dynamical scaling behaviour of the surface growth via computer simulation with various system sizes and probability P. We find that there is a transition: above a probability P_c the scaling exponent β increases rapidly, which corresponds to the change of the morphological structure in the system.

The arrangement of this paper is as follows. In section 2, the ballistic-like deposition model and the physical motivations are presented. In section 3, the dynamical scaling behaviour of the surface width and the results are discussed. The morphological structural phase transition is discussed in section 4. Finally, a conclusion is given in the last section.

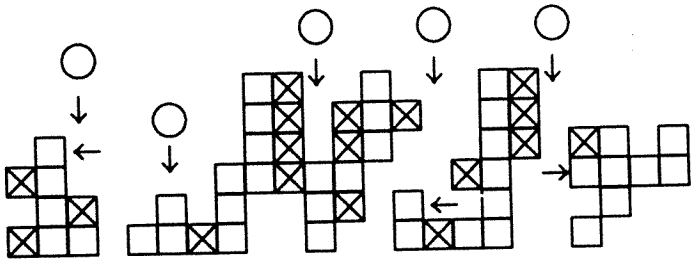


Figure 1. The ballistic-like deposition model of two kinds of particle. The circles represent the falling particles (particle A or particle C), the squares represent particle A and the squares with a cross denote particle C. The vertical arrows show the falling direction and the right- and left-pointing arrows show the positions where the falling particles may stick.

2. A ballistic-like deposition model for two kinds of particle

Two different kinds of particle, particle A (the active particle) with a probability $1-P$ and particle C (the nonactive particle) with a probability P, are deposited on a two-dimensional substrate. The particles are allowed to fall straight down randomly, one at a time, onto a growing surface. At first a column (or site) (i, j) is selected randomly, and then a particle A (or particle C) is deposited on the surface of the aggregation with a probability $1-P$ (or P). The deposition occurs once the dropping particle first encounters a particle A wherever it is—on the top or in one of the neighbouring columns of the chosen column. For instance, if the dropping particle falls down along column (i, j), and it first meets a particle A which is at the top of column (i, j) or at the top of one of the four nearest-neighbouring columns $(i+1, j)$, $(i-1, j)$, $(i, j+1)$ and $(i, j-1)$, then this dropping particle sticks to the particle A on the top of the column (i, j) or it sticks to the side of the particle A of the neighbouring column, and the falling stops. That is, the deposition not only happens on the top of the chosen column, but also on the side of nearest-neighbouring columns. When the falling particle first meets a particle C on a neighbouring column, it can fall continuously until it meets a particle A if it has not reached the top of the on-site column. In addition, if the particle first meets a particle C on the top of the on-site column, it is allowed to choose a direction at random and then continues to fall down until it finds a particle A; otherwise this particle is abandoned. For this case there is another situation: if a particle falls on a C particle with no lower neighbouring columns, this particle is also abandoned. The deposition rules are depicted in figure 1.

The continuous falling-down process of a particle might be considered as a kind of diffusion. However, this diffusion is weak for small probability P since the number of incoming particles C is small and it is easier for the incoming particle to find a particle A, and is strong for large probability P because of the large number of particles C located on the surface of or inside the columns.

The physical motivations for such model are as follows. First, it describes chemical reactions which take place on the growing surfaces of materials. For example, it models

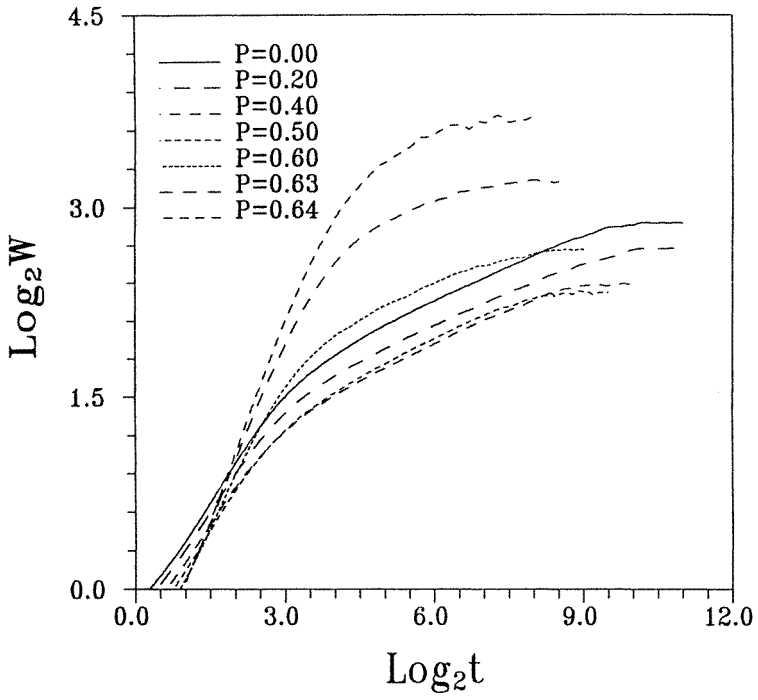
the reaction process $A + B = C$ where particle A and particle B are active. Once particle A is touched by particle B, the combination produces a product C which is no longer active. The particle A is chosen with a probability $1 - P$, and the particle B with probability P, i.e., the reactant C is produced with the probability P when P is small. Thus, in this system, some of the surface sites continue to react while some sites do not. Second, it represents the surface growth of a material with a low concentration of impurities. These impurities are represented by particle C which has bonds that are less active than those of particle A. Third, it describes the deposition of two kinds of particle (one heavy and one light) with different attractive forces. Finally, the surface growth processes of the particles on the aggregation might be considered as a kind of percolation of the particles (see [25] and references therein). The deposition of particle A introduces connective bonds for the incoming particles A and C, while the deposited particle C 'forbids' both particle A and C to stick to it. The surface keeps growing as long as the surface sites are not entirely covered by the nonactive particle C.

When $P = 0$, our model is reduced to the usual ballistic model with only one kind of particle involved and it has been studied extensively in $1 + 1$ and $2 + 1$ dimensions [1, 17, 18, 22]. The surface growth shows a dynamical scaling behaviour which belongs to the KPZ universality class. On the other hand, for $P = 1$ the surface will become completely inert after deposition of one layer of particles—that is, the particles C will cover the initial surface entirely and no growth occurs. When $P \neq 0$, the deposition process will be affected by the existence of the particles C, and there will be a diffusion of the particles which results from the disregard of the existence of particles C by the incoming particles. It is this diffusion that makes the kinetic growth of the surface and dynamical scaling exponents quite different from that in the standard ballistic deposition model, and may result in different morphological structures as we have found in the $(1+1)$-dimensional case [24]. Physically, between these two limits of $P = 0$ and $P = 1$, a percolation threshold $1 - P_c$ is expected to exist for the particle A such that for $P < P_c$, the aggregation can grow indefinitely, and for $P > P_c$, the cluster of particle A will be restricted to being small.

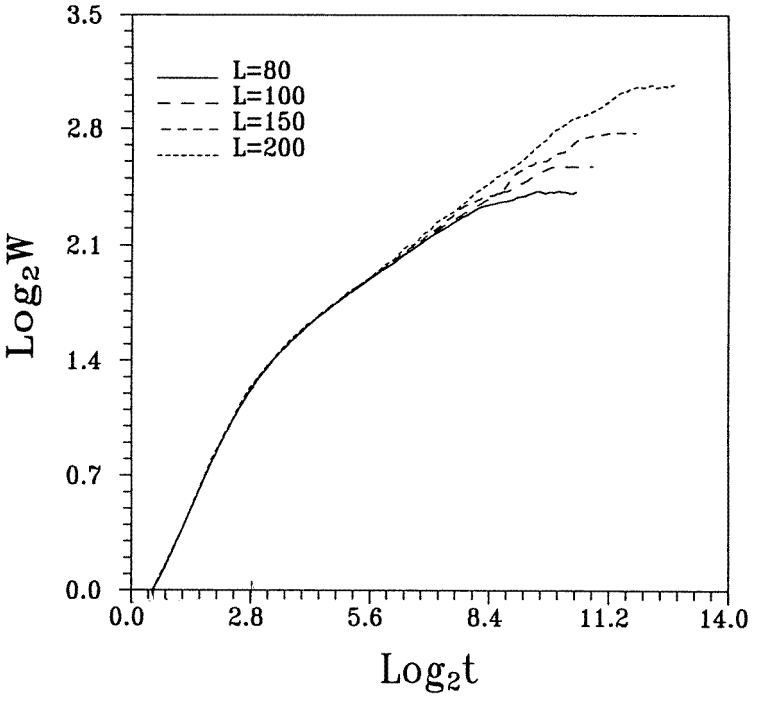
3. Dynamical scaling behaviour

Consider a square substrate of side L. The aggregation occurs in the Z-direction. At the beginning, all sites are occupied by particles A for $Z \leqslant 0$. Periodic boundary conditions are used in both the X- and Y-directions. The statistical average is obtained over 500 independent simulations for each parameter. We find that when the system size $L < 70$, the surface width W has a size dependence at the early time. This results clearly from the feature that the system size L is too small. Thus, in this work we always use a system size $L \geqslant 80$.

Figure 2 shows a log–log plot of the surface width W as a function of time t (the numbers of deposited particles) for different values of the deposition probability P and fixed system size $L = 100$ (figure 2(a)), and for different system sizes L and fixed probability $P = 0.3$ (figure 2(b)), respectively. From figure 2(a), we see the usual ballistic deposition (solid line), i.e., the ballistic deposition of only one kind of particle (particle A) or $P = 0$. The width of the surface first increases very fast, and then experiences a slowing down, and finally saturates to a fixed value. The scaling result for the exponent β is the same as obtained by previous authors [17, 21], that is $\beta = 0.238 \pm 0.005$. For $P \neq 0$ and small P, the surface width becomes smaller as the probability P increases and the saturation state is reached early. However, for $P > 0.5$ the surface width increases more rapidly as the time increases, and the system saturates much faster. These features can be clearly seen



(a)



(b)

Figure 2. The logarithm of the surface width, $\log_2 W(t)$, versus the logarithm of time, $\log_2 t$, for (a): system size $L = 100$; (b): probability $P = 0.3$.

from figure 2(a); before $P = 0.5$ the curves are below that for $P = 0$ and above it for $P > 0.5$. We define this probability as a transition probability P_c, with $P_c = 0.5$. Its physical explanation will be discussed in section 4.

From figure 2(b), we can see that the saturated widths of the surface are different for different system sizes. The growth of the surface for short times is the same. But for large values of L, the system takes a long time to reach the saturated state. From the scaling of the saturated surface width with system size, $W(t = \infty) \sim L^{\alpha}$, we can obtain the roughness exponent α. For two different probabilities $P = 0.3$ and $P = 0.6$ which are values of the probability P lower and higher than P_c, the exponent α has been calculated to be $\alpha = 0.37 \pm 0.04$ and $\alpha' = 0.30 \pm 0.03$, respectively. This gives two different values of the roughness with $\alpha > \alpha'$ which may indicate that the surface for $P < P_c$ is smoother than that when $P > P_c$. We also find that the exponents α and β obtained in our model satisfy the KPZ scaling law $\alpha + z = 2$ within 4% for $P < P_c$, but it is not obeyed for $P > P_c$.

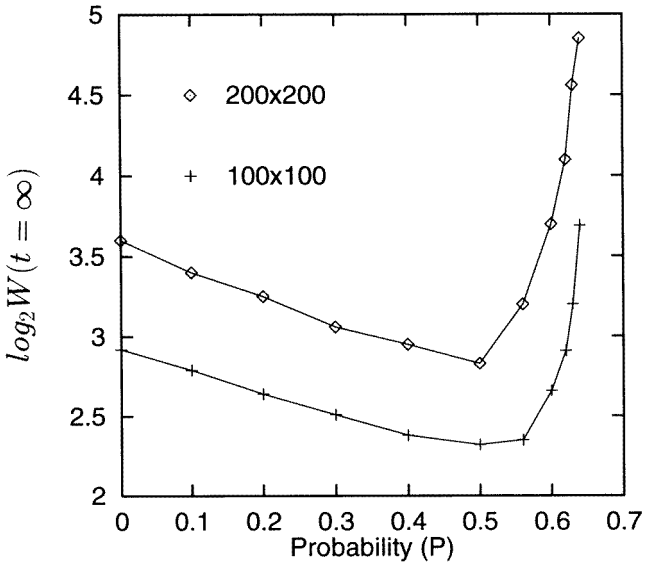


Figure 3. The logarithm of the saturated surface width, $\log_2 W(t = \infty)$, versus the probability P for two different system sizes $L = 100$ and $L = 200$.

In figure 3, we plot the saturated surface width versus the probability P for two different system sizes. We can see that the saturated width varying with the probability P shows a nonmonotonic relationship—that is, $W(t = \infty)$ first decreasing and then increasing as the probability P increases. The values of the probabilities of the minimal points are around 0.5, i.e., $P_c \simeq 0.5$ for both cases of different system sizes. It is worth noting that in figure 3, we have included the values of the saturated width for $P = 0$. As we can see, these saturated widths are $\log_2 W(t = \infty) = 2.88$ and 3.63 for $L = 100$ and 200, respectively. They are just on the lines shown in figure 3. This strongly supports a monotonic decrease of the saturated width with respect to the probability P.

We have also plotted the exponents β as a function of the probability P, and for $P < P_c$ we find that β is almost unchanged with increasing probability P, and increases rapidly after P_c has been reached (see figure 4). Notice that the definition for the value of the transition probability P_c here is slightly rough. For a more precise definition, one must study the critical behaviour (see the following discussion).

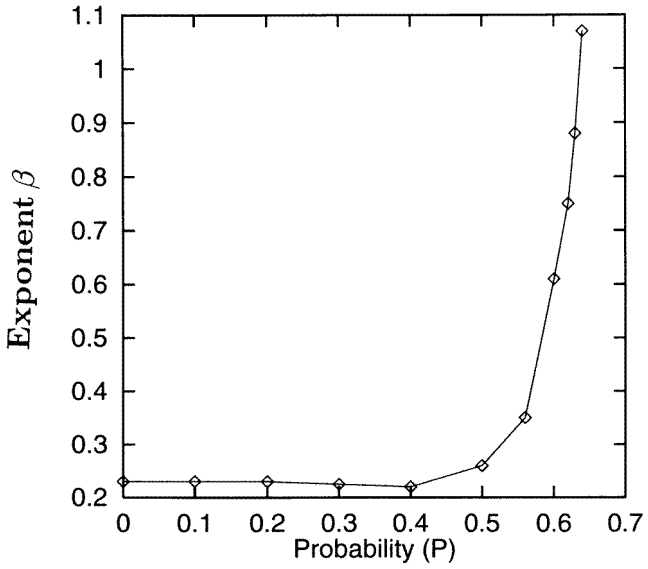
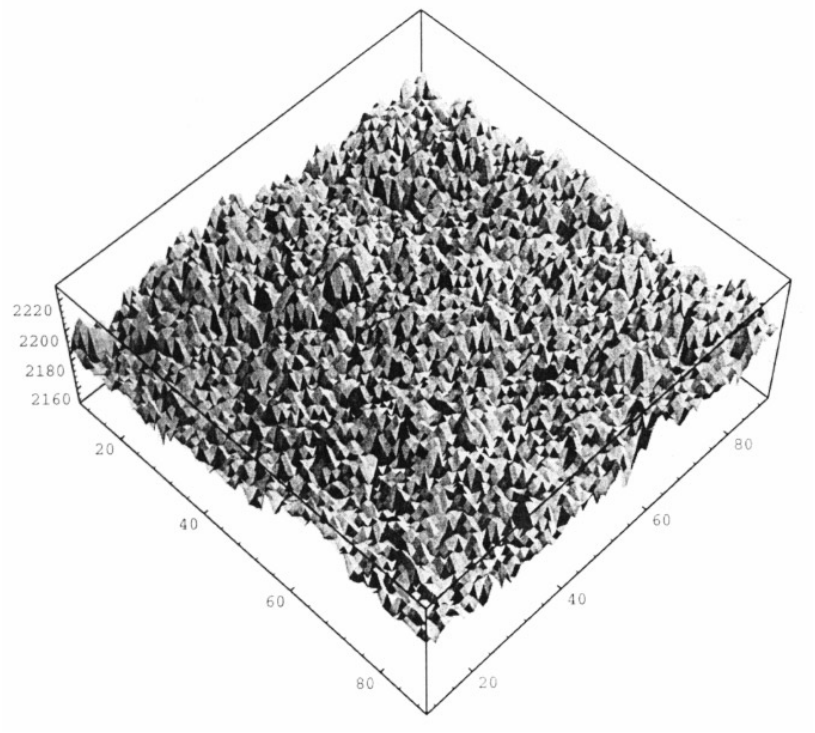


Figure 4. The scaled exponent β at early times of the surface growth against the probability P.

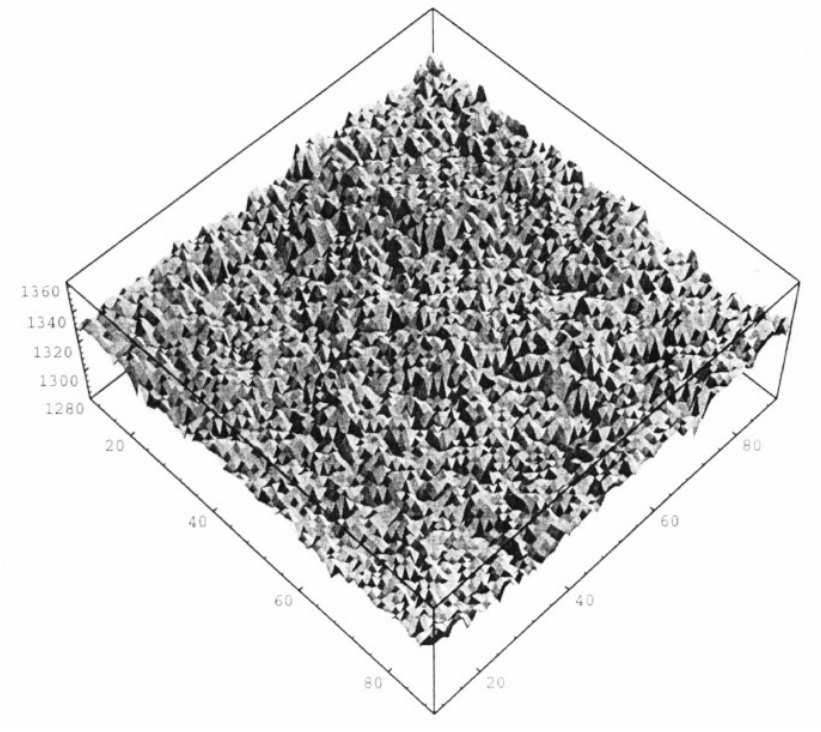
4. A morphological structural phase transition

From the discussion in the last section, we see that for the ballistic-like deposition model the dynamical scaling behaviour shows us that as the probability of deposition of particle C increases, there exist two different scaling regions separated by $P_c = 0.5$. We define this as a transition in the morphological structure. This kind of phase transition is due to a special diffusion process which results in a directed percolation of the active state. For $P > P_c$, the nonactive particles tend to connect themselves to form a large inert cluster, which blocks the connection of the active cluster of particle A. Therefore, the morphological structures are different when the deposition probability is below or above its critical value P_c.

Figure 5 shows the shapes of the surface. We see that the surface is locally rough and on average the differences in heights between the valleys and the peaks are not very big for $P < P_c$ (see figure 5(a) and 5(b)). When $P > P_c$, the surface is dominated mainly by relatively large terraces, and the terraces have a large difference in heights as shown in figure 5(c). Microscopically, the formation of such different morphological structures can be understood as follows: for small P, the deposition of particle A occurs more frequently and these depositions form a lot of barriers locally which block the continued falling down of particles, and the particles have more chances to attach to the sides of the columns and overhang is produced more easily. Thus a local valley between columns may be connected because of the overhang and the differences in heights between the columns are small, which makes the surface appear morphologically rough down to short length scales. At the same time the structure below the surface is less compact; there are many holes under the surface due to the overhang that arises. Nevertheless, for $P > P_c$, the influx is dominated by particle C, while the overhang of particles is more difficult to produce. Therefore the deposition of particles A and C has a high probability of being located on the terraces once these terraces have been formed. The difference in heights between the terraces is large. From the continuous falling of particle C it looks like particles C aggregate together to form

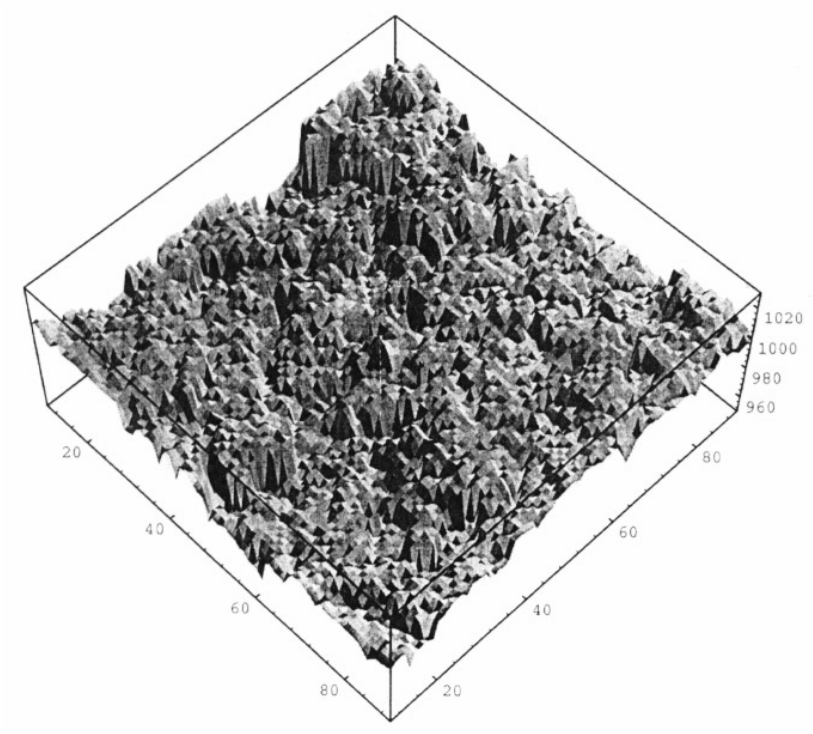


(a)



(b)

Figure 5. See facing page.



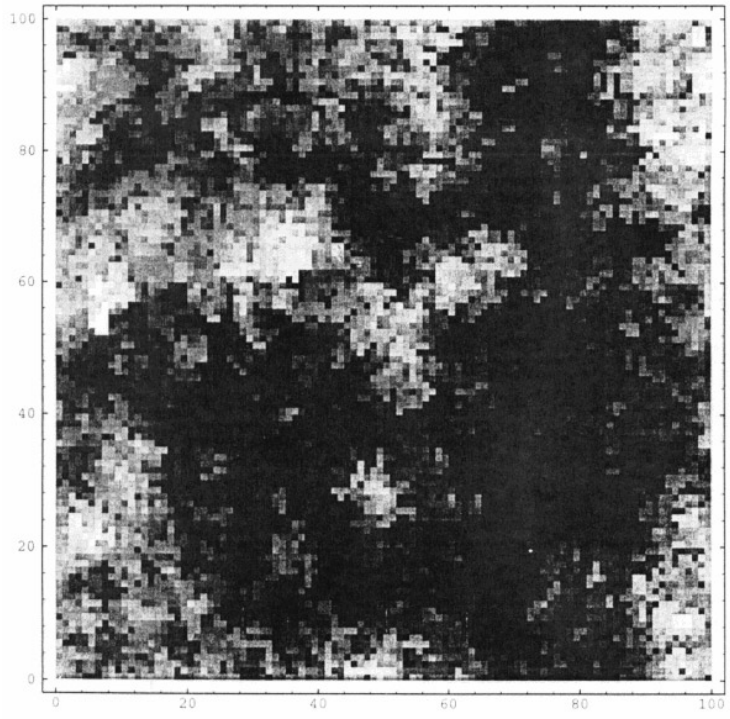
(c)

Figure 5. Three-dimensional plots for the shapes of the surface with different probabilities P for the saturated states: (a), $P = 0$; (b), $P = 0.5$; (c) $P = 0.63$.

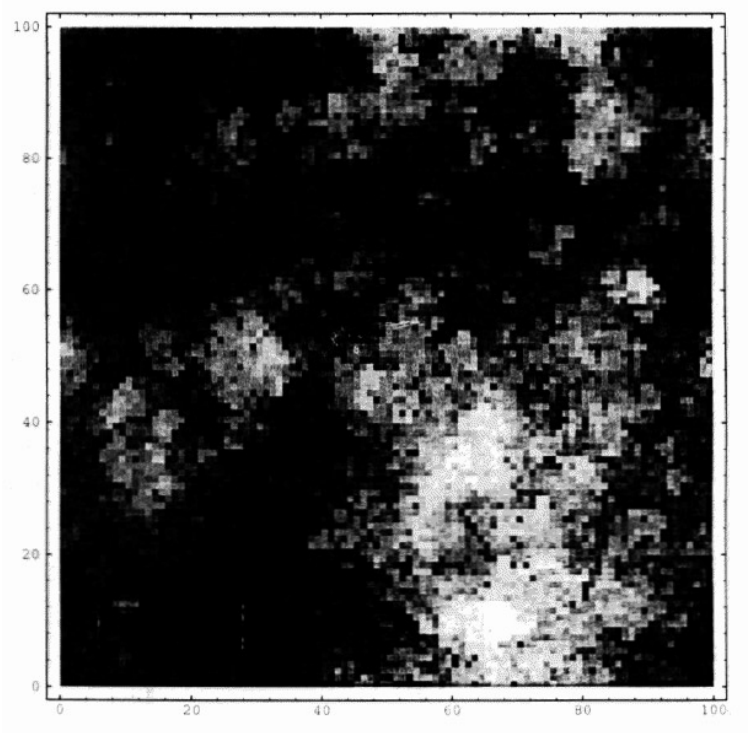
big clusters.

In figures 6, we show plots of the density of the particles in the system. White areas represent particles C, dark areas represent particles A, while grey gives an idea of the height of the column. It is clear that for $P < P_c$ the particle distribution of both A and C is basically uniform and the sizes of the clusters of particle A are big (see figure 6(a) and 6(b)), while for $P > P_c$ the terraces are clearly seen and the sizes of the clusters of particle A are small (cf. figure 6(c)). Furthermore, in order to verify the above, we have also counted the number of particles C, N_c, on the surface as shown in figure 7. We found that N_c has a linear relationship with the probability P, having different slopes before and after the transition. Actually, when we observe the density of particles C as a function of the probability for the whole aggregation, it will also show a similar change below and above P_c.

All of the above discussions indicate that there exists a morphological structural phase transition in the surface growth by ballistic-like deposition. Comparing these results with that of [24], for the $(1+1)$-dimensional case, the transition is more apparent due to stronger diffusion of particles C, which is enhanced by the second spatial direction. The surface growth has a higher upper limit value of the probability P, P_{up}, for the complete stopping of the growth, i.e, disappearance of the bonding sites beyond P_{up}. It has been found that this value is shifted from $P = 0.35$ for the $(1+1)$-dimensional case to $P = 0.65$ for the present $(2+1)$-dimensional case. In the $(1+1)$-dimensional case, we found it difficult to find convincing evidence that there is a such phase transition since the range of the probability

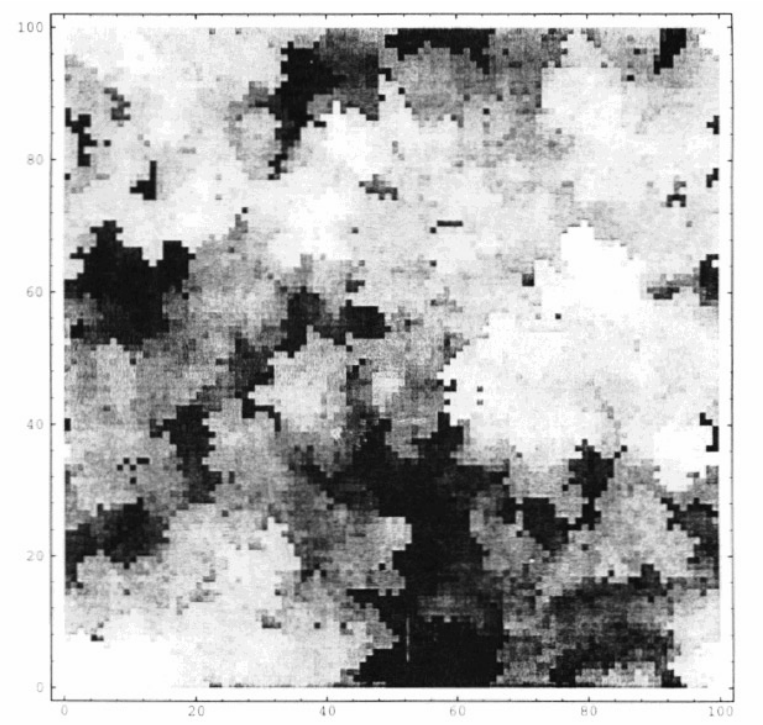


(a)



(b)

Figure 6. See facing page.



(c)

Figure 6. The density plots for system at the saturated states, with the white area for particle C, the dark area for particle A, and the grey area for the height of the column. (a) $P = 0$; (b) $P = 0.5$; (c) $P = 0.63$.

of deposition studied is much narrower and the scaling behaviour of the saturation surface width and the exponent with the probability is not so apparent. However, in the present case, the deposition probability has a wider range and the exponent β clearly varies a lot above the transition.

Physically, the morphological transition studied in the present paper corresponds to a change from an active state to an inert state, which could be described by directed percolation theory. Evidence for this is the appearance of large clusters of particle C sites on the surface around P_c. For $P < P_c$, the falling particle (A or C) connects to a particle A easily. The surface grows continuously and a directed percolating cluster (particle A) extends over the whole system. For $P > P_c$, a typical connected particle A cluster extends over a small distance, i.e., the connected particle C cluster will extend over the entire system. As a result, this directed percolating process governs the growth of the surface microscopically, which makes the surface structures different from each other for the probability P below and above P_c.

5. Conclusion

Before concluding, it is worth making a remark on the scaling exponents. In our simulations, we have obtained various exponents β and α for different probabilities. For values of the

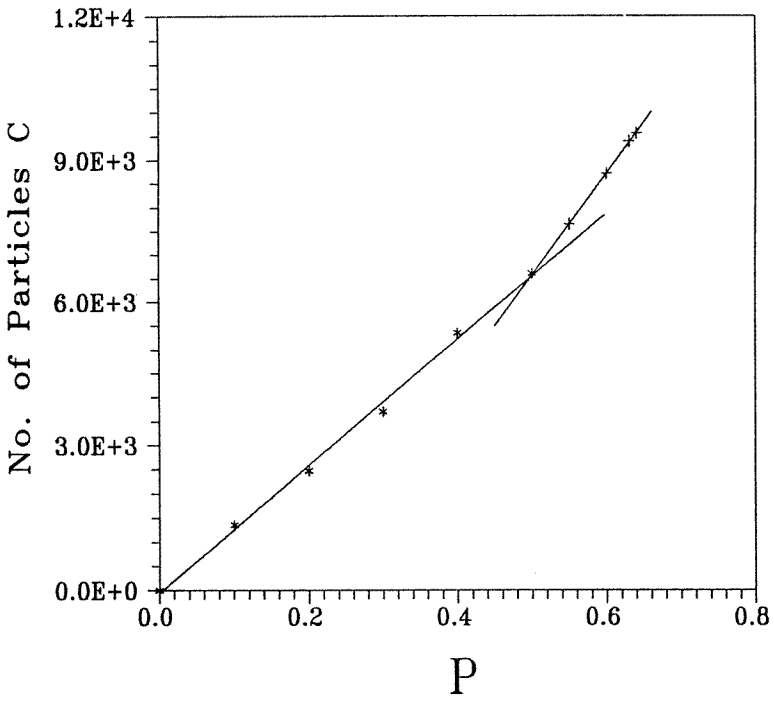


Figure 7. The number of particles C on the surface in the saturated state against the probability P for the system size $L = 100$.

probability $P < P_c$, we find that they satisfy the KPZ scaling law, while they do not satisfy it for $P > P_c$. In fact, this is also due to the kinetic diffusion of the particles. For $P < P_c$, the local distribution of particles is dominated by the active particle A; the incoming particles A or C basically do not need to diffuse, and they can easily stick to the surface. Thus, the 'interaction' between the particles is strong, and the nonlinearity in the growing processes due to diffusion and local geometric symmetry is weak, and the model is close to the usual ballistic deposition model. The scaling exponents β and α, of course have values similar to those of the usual ballistic deposition model which has been found to fall in the KPZ universality class. The situation will become different as the probability increases. The local positions on the tops of the columns or inside the columns have a high probability of being occupied by particles C which forces the incoming particle to diffuse before deposition. This introduces a weak 'interaction' between the particles, which makes the kinetics of growth different from that of the usual ballistic deposition model. Therefore the scaling exponents β and α will no longer follow the KPZ scaling law. This means that the continuum KPZ equation does not apply to this case for the parameter range $P > P_c$.

From the changes in the surface morphological structures and the sticking rules of the particles, we could interpret our results in terms of the directed percolation theory. In fact, the relationship between the roughness of the surface of the growing aggregation and the percolation behaviour could be explained in terms of the power-law behaviour of the correlation length and the steady-state velocity of the surface growth. Since we are only interested in the dynamical scaling of surface growth at early times and report a possible morphological structural transition in this new model, we did not study the

critical behaviour around the transition. For a complete understanding of the kinetics and the percolation behaviour, much more detailed work, such as a study on the relationship between the roughness exponent and the growth velocity as a function of the probability P for long times, and the characterization for the critical behaviour, is needed. We will report this in the following work.

In conclusion, we have proposed a new ballistic-like surface growth model for deposition of two kinds of particle (A and C) on a two-dimensional substrate. We have obtained the scaling behaviour of the surface width W for different values of the probability P of particle C and system sizes. We find that there is a phase transition of the morphological structures as the probability increases. This transition is defined by the exponent β as a function of the probability P. We argue that the physical origin of the transition lies in the diffusion of the particle which passes through the less active particle C without reaction with it. It is the kinetic diffusion and the interaction between the two kinds of particle that results in the growth of the surface through the directed percolation process. The morphological structural transition could be interpreted as a transition from an active state to an inert state.

Acknowledgments

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