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Ballistic deposition model for multiple species with next nearest-neighbour interactions in (2+1)-dimensions

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Abstract

The kinetics of surface growth and its morphological structure have been studied for a ballistic deposition-like model with two kinds of particles (A and C) upon extending the interaction between particles to next-nearest-neighbours. The dynamic scaling behaviour of the surface width has been obtained for different values of the deposition probability P for particle C and system sizes. A morphological structural transition has been found as the probability increases. This transition is well defined both by the scaling of the saturation value of the surface width and the velocity of growth. It has been found that the extracted values for the roughness and growth exponents, for different values of P, do not obey the scaling law given by the Kardar–Parisi–Zhang equation. © 1997 Elsevier Science B.V.

Keywords: Computer simulations; Dendritic and/or fractile surfaces; Models of non-equilibrium phenomena; Models of surface kinetics

1. Introduction

Recently, the growth and formation of surfaces and interfaces have attracted great interest due to their importance in material sciences and the relevance in understanding nonequilibrium statistical mechanics [1,2]. It is well known that a stochastically growing surface exhibits scaling behaviour and evolves to a steady state without a characteristic time or length scale. This has led to the development of the dynamical scaling approach proposed by Family and Viscek [3]. Starting with an initially flat substrate, defining the surface width $W(L, t)$ by

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

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 average of the surface height, the scaling law is given by

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

The dynamical scaling behaviour is characterized by the roughness exponent α and the dynamical exponent z, with growth exponent $\beta = \alpha/z$. The function $f(x)$ scales as $f(x) = x^{\beta}$ for $x \ll 1$ and $f(x) =$

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constant for $x \gg 1$. This scaling behaviour has been studied in a wide variety of models and experiments [4] and has been argued to be universal [1,2]. One successful theoretical approach is the Kardar–Parisi–Zhang (KPZ) approach [5] which is based on Edwards and Wilkinson's theory [6]. The KPZ equation is a nonlinear Langevin equation

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

In (1+1)-dimensions, i.e. $d=2$, Eq. (3) can be solved analytically giving $\alpha = 1/2$ and $\beta = 1/3$. These results are in good agreement with the results obtained from the simulation of ballistic deposition and Eden models [5,7]. However, for $d>2$ there is still disagreement over the values of the exponents as well as the universalities of the various surface growth models [8,9]. In addition, dynamic renormalization group analysis indicated the possibility of a nonequilibrium roughening transition from the weak-coupling to a strong-coupling regime for $d > d_c = 2$. It has also been suggested that anomalous roughening behaviour may arise at the transition. Several authors have tackled the problem of growth models for various dimensions [10–16] and it has been found that there is a phase transition which 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 structural transition will appear in general. The study of discrete models may provide new insight into the dynamics of the surface growth for $d>2$.

Among the growth models which give rough surfaces, a well-studied example is the ballistic deposition model [17]. Here 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 compact. All previous work, which has been carried out according to the model described above, concerned only the growth of one kind of particle [1,2,16]. In general the growth of real materials may contain different kinds of particles. Thus, in the growing system, there may exist different interactions for different particles and the growing mechanism may also be different. In addition, in (2+1)-dimensions, next-nearest-neighbour (NNN) interactions have never been studied, even for one kind of particle. It has been reported before that upon changing the interaction to next-nearest-neighbours neither the exponents nor the universality class change [18]. Thus, we have carried out this study not only to understand the growth mechanism for the model with two kind of particles better, but also to extract the values of the exponents for the case when only one particle is used.

Following our previous work [9,19,20], we report further results of a ballistic deposition-like model in (2+1)-dimensions with NNN interactions. The kinetic growth of the deposition of two kinds of particles A and C with probabilities $1-P$ and P, respectively, on the substrate is described using the probability as a continuous tunable parameter to control the system. The dynamical scaling behaviour of the surface growth through computer simulation is studied with various system sizes and probability P. It has been found that there is a phase transition around a probability P_c such that the scaling exponent β increases above P_c. This corresponds to a change in the morphological structure of the system.

2. Model

As shown in Fig. 1a, two kinds of particles, particle A (the active particle) and particle C, are deposited on a two-dimensional substrate, with probability $1-P$ and P, respectively. 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 C is deposited onto the surface of the aggregate. The deposition occurs at the moment when the incoming particle first encounters a particle A, whether it is on the top or on one of the neighbouring columns of the chosen site. For instance, if the dropping particle falls down along column (i, j) and it meets a particle A which is at the top of the column (i, j) or at the top of one of the eight neighbouring columns as shown in

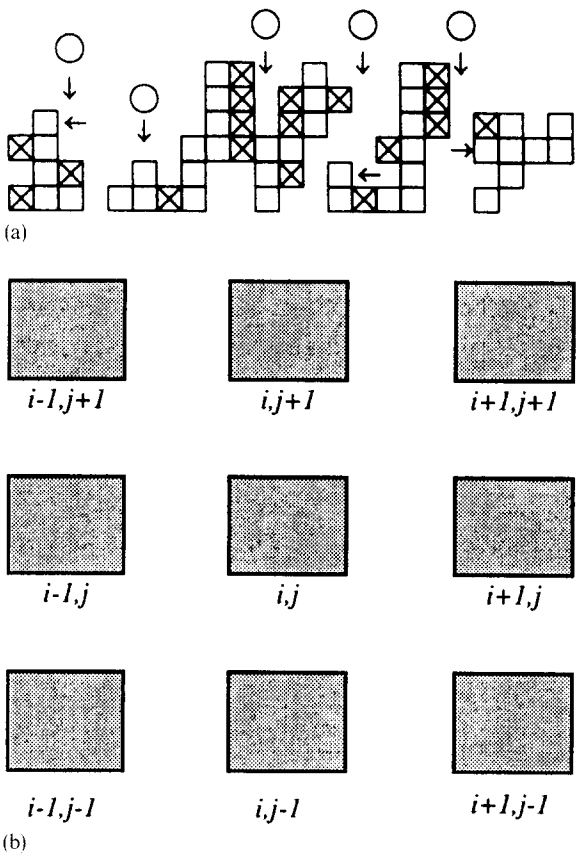


Fig. 1. (a) The ballistic-like deposition model of two kinds of particles. The circles represent the falling particles, the squares represent particles A and the squares with a cross denote particles C. (b) The eight neighbours for the chosen site i, j.

Fig. 1b, this dropping particle sticks to this particle A and stops falling. That is, the deposition not only happens on the top of the chosen column, but also on the side of the nearest- and next-nearest-neighbouring columns. When the falling particle first meets a particle C on neighbouring columns, it may fall down until it meets a particle A or it reaches the top of the on-site column. This falling down of the incoming particles could happen only if the chosen site has a lower height than its neighbours and all its neighbours contain particles C above the height of the on-site column. Since the growth of any column in this case depends on eight neighbours and there are different interactions between particles, the deposition process is not easy to imagine from Fig. 1, which gives a simple side view of this model.

The physical motivations of such a model are as follows: first, it describes chemical reactions which take place on the growing surface of materials. For example, we model the reaction process $A+B=C$ where particles A and 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 P. That is, 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 low concentration of impurities. These impurities are represented by particle C which have less active bonds than particle A. Third, it describes the deposition of two kinds of particles (one heavy and one light) with different attractive forces. Finally, the surface growth processes of the particles on the aggregate might be considered as a kind of percolation of the particles [21]. The deposition of particles A introduces connective bonds for the incoming particles A and C, while the deposited particle C forbids both particles A and C from sticking 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 a single kind of particle. The ballistic model, with one kind of particle with next-nearest-neighbour interactions, has only been studied in $(1+1)$-dimensions for a restricted solid-on-solid (RSOS) model [22]. When $P\neq 0$, the deposition process will be affected by the existence of the particle C, and competition will exist between both processes: downward diffusion and overhangs. For downward diffusion the chosen site has to be lower than its neighbours. If one of the neighbours is particle A, then the incoming particle will stick to it, thus overhanging. If they are all Cs, the particle will continue downwards until it finds a particle A on a neighbour or on the chosen site. Otherwise it is abandoned, thus simulating desorption. These processes, which come from the different interactions between particles, make the kinetics of the growing surface and the dynamical scaling behaviour quite different and may result in

different morphologic structures. For $P=1$, the surface will become completely inert after deposition of one layer, i.e. the particles C will cover all the surface and no growth will occur.

3. Simulation results

The aggregation occurs in the Z-direction over a square substrate of side L. At the beginning, all sites are occupied by particles A for $Z \leq 0$. Periodic boundary conditions are used in both the X- and Y-directions. The statistical average is obtained over 500 independent simulations for each parameter.

Fig. 2 shows a log–log plot of the surface width W as a function of time t, where t is measured as one Monte-Carlo step, for different values of the deposition probability P and fixed system size $L=100$ (Fig. 2(a)) and for different system sizes L and fixed probability $P=0.3$ (Fig. 2(b)), respectively. As indicated in Fig. 2(a), the width of the surface first increases very fast and then experiences a slowing down, finally saturating to a fixed value. For $P \neq 0$ and small values of P, the surface width becomes smaller as the probability P increases and the saturation state is reached for smaller values of the width. However, for $P>0.5$ the surface width increases again as the time increases and the system saturates faster. So, we define the probability $P=0.5$ as a transition probability P_c. Fig. 2(b) shows the surface width for different system sizes for $P=0.3$. The growth of the surface for short time is the same. With large values of L, the system takes a long time to reach saturation. From the scaling relation of the saturated surface width with system size, $W(t=\infty) \sim L^{\alpha}$, the roughness exponent is obtained for two different probabilities below and above P_c, $\alpha=0.25\pm0.03$ and $\alpha'=0.32\pm0.02$ for $P=0.3$ and 0.7, respectively. This gives two different values of the roughness with $\alpha<\alpha'$, which may indicate that the surface for $P<P_c$ is more jagged than that for $P>P_c$. Also, we found that when $P=0$, the roughness exponent $\alpha_0=0.21\pm0.03$.

The saturated surface width versus the probability for fixed value of the system size is shown in Fig. 3. According to this figure the saturated width first decreases upon increasing the probability $P<0.5$ and then increased with $P>0.5$. The value of the probabilities of the minimal point is around 0.5, i.e. $P_c \approx 0.5$.

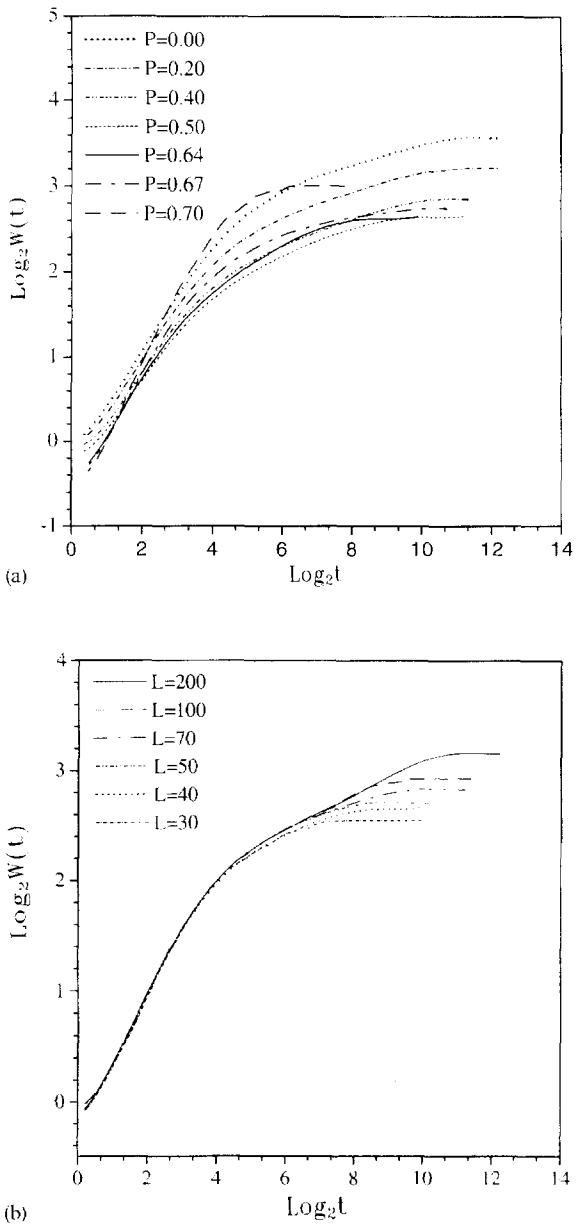


Fig. 2. (a) $\log_2 W(t)$ versus $\log_2 t$ for a system size $L=100$. (b) $\log_2 W(t)$ versus $\log_2 t$ for a probability $P=0.3$.

The exponent β is plotted as a function of the probability P as shown in Fig. 4. It has been found that β is almost unchanged with increasing P for

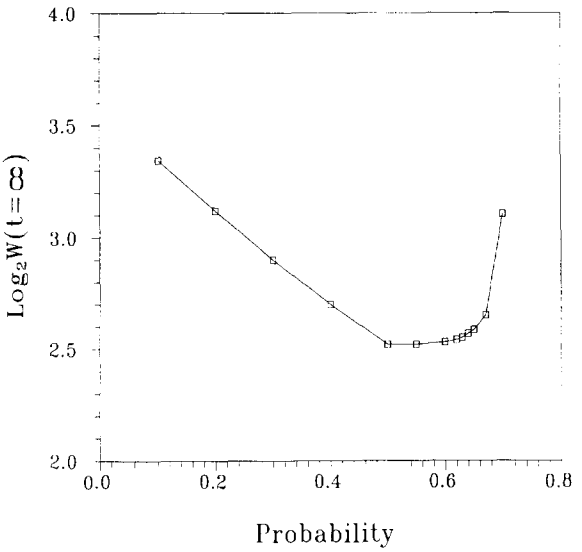


Fig. 3. $\log_2 W(t=\infty)$ versus P for system size $L=100$; the solid line joining the calculated points is drawn for convenience.

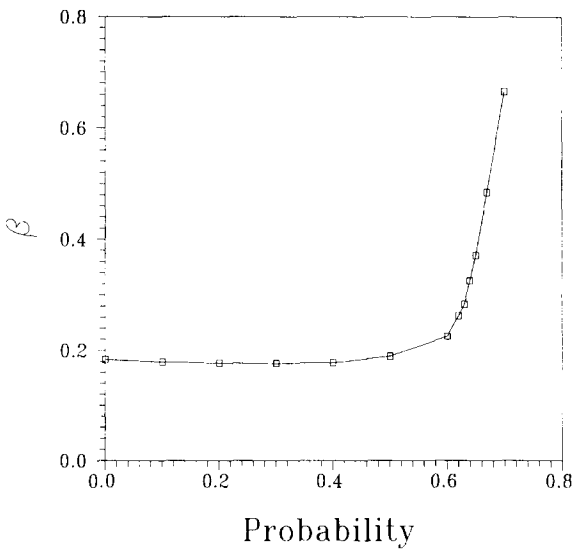


Fig. 4. The exponent β against the probability P; the solid line connecting the calculated points is drawn for convenience.

$P<P_c$ and then increases rapidly after P_c but it does not reach the value of 1. The values of β for $P<P_c$ and $P=0$ are found to be around 0.2, which are different from $\beta=0.25$ for the ballistic deposition model with nearest-neighbour interactions only [8]. Here the calculated error is smaller than the difference. Also, the values of the exponents α and β do not obey the scaling law $\alpha+\alpha/\beta=2$ either below or above P_c. This scaling law is characteristic of standard KPZ theory and its extensions [5,7].

It is well known for the ballistic deposition model that the interface advances with time in a nonuniform way, i.e. the average interface velocity does not equal zero [8]. It is clear from Fig. 2 that a decrease exists and a rapid increase in the values of the saturated surface widths for probabilities lower and higher than P_c, respectively. Also after P_c, the surface width grows very fast with time associated with a higher value of β and saturation is reached in a short time. Therefore, the study of the interface velocity for different values of probabilities may introduce a way to elucidate this behaviour.

Fig. 5 shows the calculated interface velocity versus time for different probabilities. It can be seen from this figure that the velocity decreases with time, then slightly increases and finally reaches a constant value for each value of the probability. For values of $P\leq 0.5$, the behaviour takes the same trend as the usual ballistic model but with different values in the final stage for each, while for $P>0.5$ it changes drastically, especially

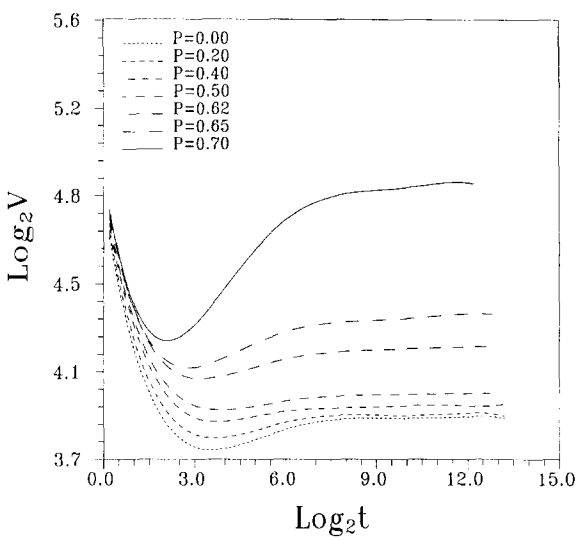


Fig. 5. The logarithm of the growth velocity versus time for different values of P.

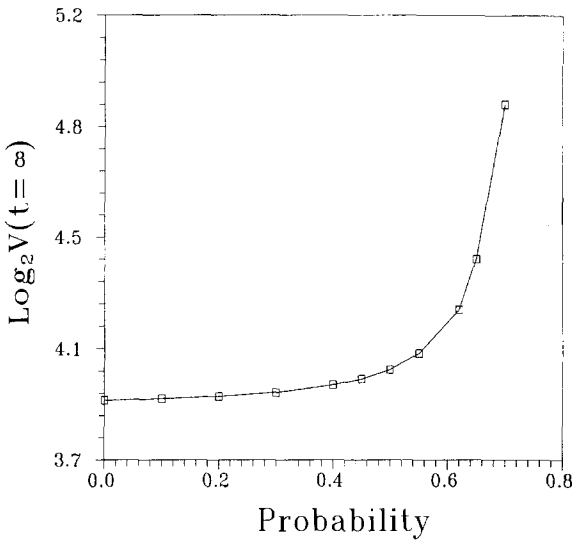


Fig. 6. The logarithm of the steady-state velocity versus probability P; the solid line joining the calculated points has been drawn for convenience.

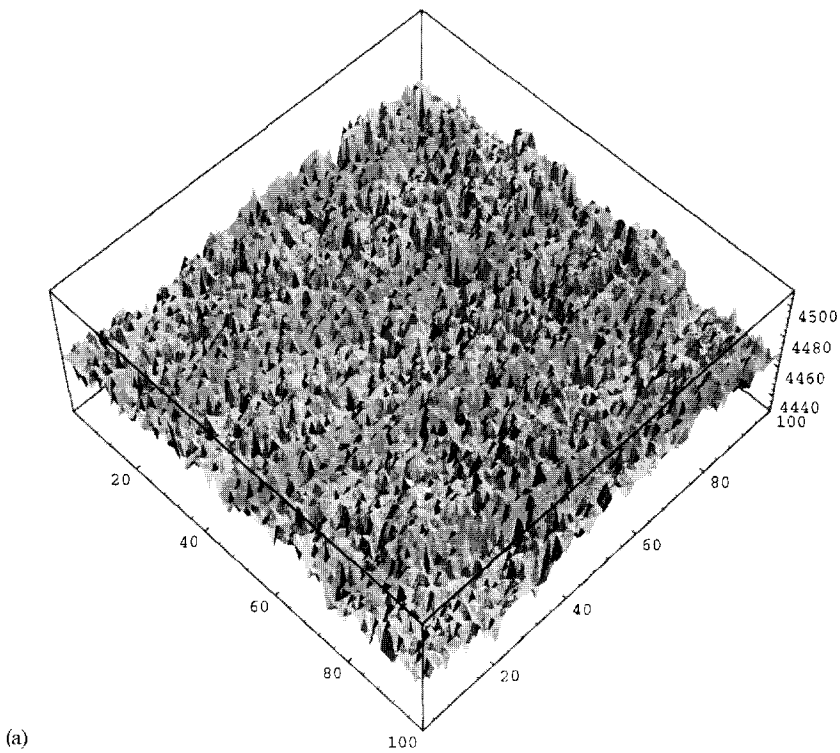
for $P>0.65$. Fig. 6 shows the steady-state velocity versus time for different values of P. This figure supports the existence of the phase transition in kinetics which should arise due to a transition in the morphological structure.

4. Morphological structural transition

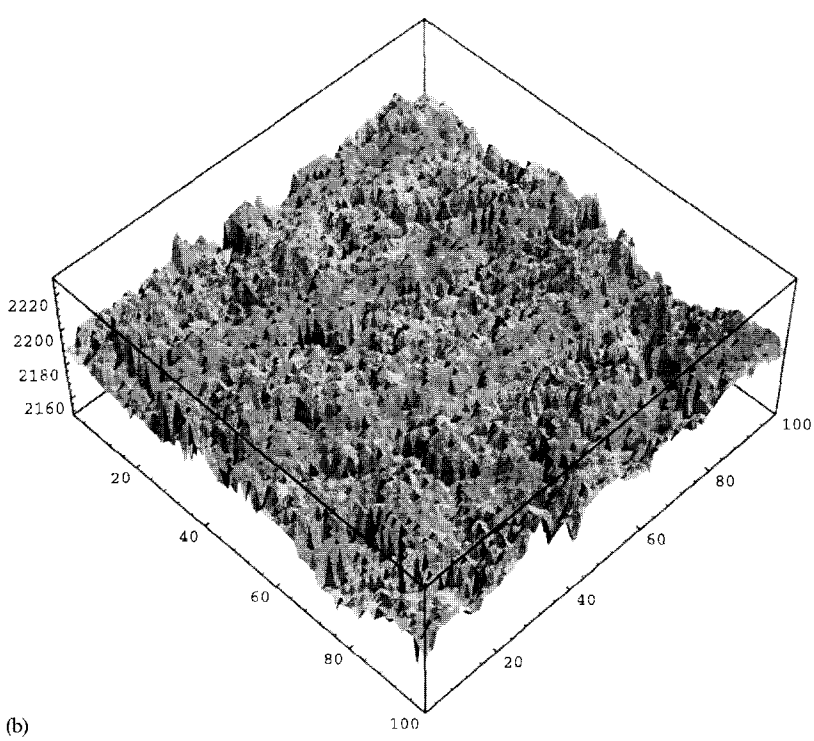
We showed in the previous section that the dynamic scaling behaviour gives us an indication that as the probability of deposition of particle C increases, two different scaling regions exist separated by $P_c=0.5$. This could be defined as a transition in the morphological structure and it is due to the interaction processes between different kinds of particles. For $P>P_c$, the nonactive particles C tend to connect themselves to form large clusters, which block the connection of the active clusters of particles A.

Fig. 7 shows the shapes of the surface at $P=0.3$ and 0.7, which gives an indication that the surface is locally rough. Comparing Fig. 7(a) with Fig. 7(b), we see that the surface at $P=0.7$ looks smoother than that at $P=0.3$, noting that the differences in height of both are the same. For $P<P_c$ the deposition of particles A occurs more frequently than that of particles C. Since the bond strength between particles A is big, they are connected together forming big clusters separated by very small islands of particles C. This may lead to rapid growth of the columns that contain particles A on their tops as well as their neighbours through the sideways sticking and a low growth of columns that contain particles C on the top or particles C on the neighbours. The process in this case may produce a rough surface with a sensible variation between its columns. For $P>P_c$, there will be more particles C than A on the top of the columns and on the neighbours. The incoming particle cannot move downwards to encounter a particle A unless the neighbours of the chosen site are covered by particles C. This must happen for all layers through which the incoming particle descends. Such a case has a small chance, as it is most probable that the incoming particle meets particle A in the second layer if it has not done so in the first. This may cause more overhanging which enhances the lateral spreading of the surface [23]. This mechanism leads to an increase in the lateral correlation length reaching the value of L fast, then the system saturates earlier in time. In fact, the effect of more overhangs is responsible for the increase of the interface velocity after P_c since it leads to the formation of voids under the surface, which in turn, increases the surface gradient. Therefore, the particles stick to the surface nonperpendicular to the local gradient which increases the nonlinearity in the growing surface.

Fig. 8 shows the density ρ of the whole aggregated materials versus the probability P, where $\rho=N/\bar{h}L^{(d-1)}$ and N is the number of particles. It is clear from this figure that upon increasing the probability P, the density of particles C increases and then decreases after $P=0.5$ and the density of particles A decreases. So, the total density of the aggregated material decreases. This supports that there are more overhanging processes than downward diffusion of particles while the surface grows. That is, the density decreases due to the formation of big voids inside the bulk which in turn becomes less compact.



(a)



(b)

Fig. 7. The three-dimensional plots for the shapes of the surface with different probability P_s: (a) $P=0.3$; (b) $P=0.7$.

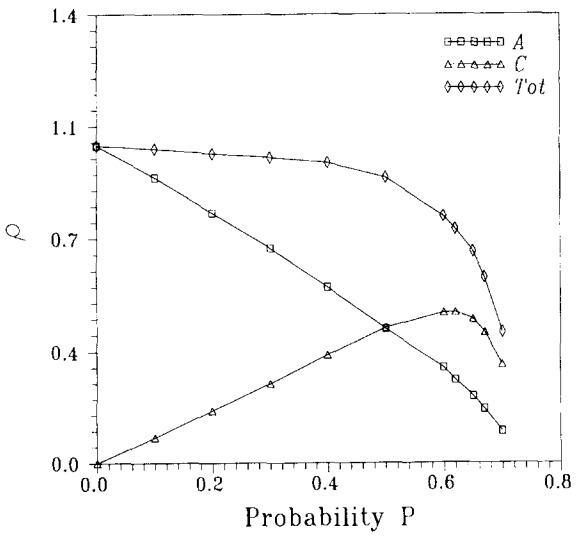


Fig. 8. The density of particles ρ against the probability P.

Fig. 9 shows density plots of the surfaces. The white areas represent the highest columns and the dark areas represent the lowest. Variation in the shades of grey gives an indication of the fluctuations of the height. It is seen from Fig. 9 that the grey variation and the contrast between columns are sharper when $P=0.3$ than when $P=0.7$. This reflects that the surface is going to be smoother for $P>P_c$. According to this and to the extracted values for the exponent β, a transition in the morphological structure occurs. Furthermore, in order to verify the above, the number of particles C, N_c, on the surface is counted and plotted against the probability P as shown in Fig. 10. It is found that N_c has a linear relationship with the probability P, having different slopes before and after the transition.

All of the above discussions indicate the existence of the morphological structural transition in the surface growth by ballistic-like deposition model. This transition corresponds to a change from an active to an inert state, which could be described by directed percolation theory. Evidence for this is the appearance of large clusters of particles C on the surface around P_c. For $P<P_c$, the falling particles (A or C) connect to particles 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 particles A cluster extends over a small distance, i.e. the cluster of connected particles C 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

In our simulations, we have obtained various exponents β and α for different probabilities. It has been found that the exponents do not satisfy the KPZ scaling law below and above P_c. This may be attributed to the facts that: (a) the inclusion of the next-nearest-neighbour interactions between particles enforces the nonlinearity in the growth processes; (b) upon increasing the probability P, more overhangs occur and wide vacancies (defects) in the bulk are formed. This may enhance the nonlinearity in the growth along these defect lines. Therefore, the continuum KPZ equation does not apply in this case.

In conclusion, a ballistic-like surface growth model for deposition of two kinds of particles on a two-dimensional substrate with next-nearest-neighbour interactions has been proposed. The dynamic scaling behaviour of the surface width W for different values of the probability P and system sizes has been obtained. A phase transition of the morphological structures has been found as the probability P increases. This transition is defined by the exponent β as a function of the probability P. The physical origin of the transition lies in the tendency of particles C to aggregate together to form inert clusters and to the different interaction processes between different particles. This results in the growth of the surface through a directed percolation process. The morphological structural transition could be interpreted as a transition from an active state to an inert state. Also the presence of particles C leads to void formation and accordingly a rapid increase in the lateral correlations.

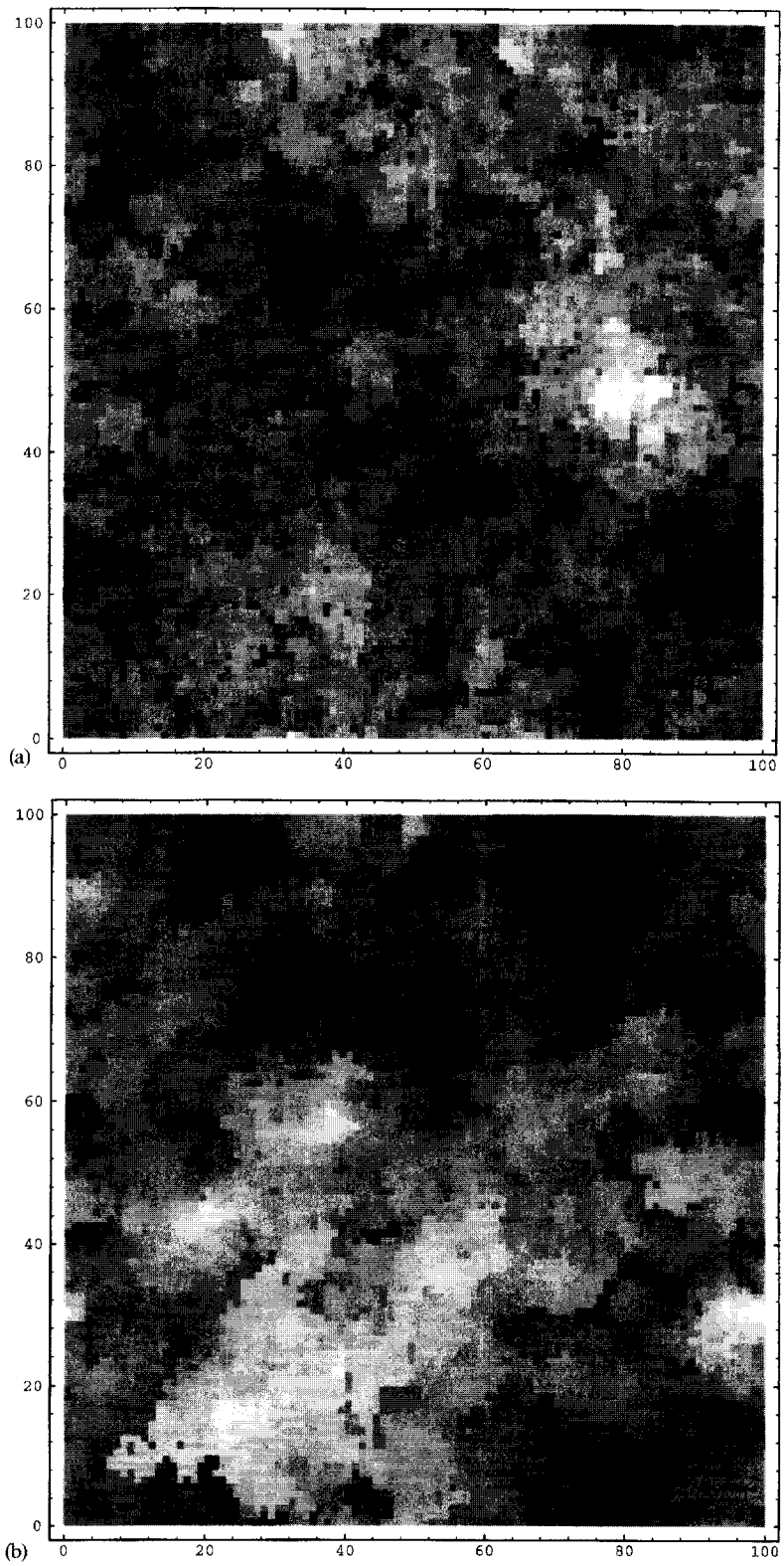


Fig. 9. The density plot of the variation of the heights of the columns: (a) $P=0.3$; (b) $P=0.7$.

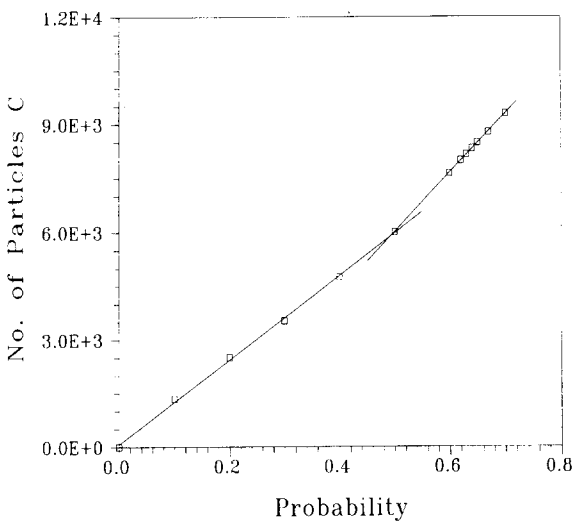


Fig. 10. The number of particles C on the surface against the probability P for the system size $L=100$. It is clear that there is a distinctive difference in the slope of the curve below and above P_c.

This effect induces the growth rate to reach saturation at earlier times with higher speed.

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