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Random deposition-like model for two species in (2+1) dimensions

Hassan F. El-Nashar [a], Hilda A. Cerdeira [b]

[a] Department of Physics, Faculty of Science, Ain Shams University, Abbassia, Cairo, 11566, Egypt
[b] The International Center for Theoretical Physics, P.O. Box 586 34100 Trieste, Italy

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Abstract

We present a random deposition-like model in (2+1) dimensions for two kinds of interacting particles A and C. The dynamical scaling behaviour shows a growth exponent β as a function of P, where P is the probability of being a particle C. The morphologic study reveals a system instability for small values of P. It also indicates that the presence of C particles leads to interface pinning. The results suggest that the model does not belong to the Edwards–Wilkinson universality class.

Keywords: Growth; Models of non-equilibrium phenomena; Models of surface kinetics; Surface diffusion

1. Introduction

The growth of surfaces and interfaces has attracted interest not only because of its importance in technology but also because of its relevance for understanding non-equilibrium statistical mechanics [1,2]. It is well known that a stochastic 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 [3]. Starting with initially flat substrate, defining the surface width $W(L, t)$ by

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

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 takes the form

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

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 $x<1$ and $f(x)=$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].

It is common in growth processes to find local diffusion of the newly arriving particles along the surface of the deposited material. Surface diffusion leads to surface relaxation and its effect is similar to that of surface tension in liquids [1]. Recently, a variety of models have been introduced in order to incorporate such effect into surface growth models [1,2,4]; the deposited particle is allowed

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to move on the surface within a finite distance from the column in which it was fallen until it sticks on a column of minimal height and becomes a part of the aggregate. In this case surface diffusion introduces non-trivial correlations between different columns. Computer simulations indicate that in (1+1) dimensions, the surface width grows with time as $W(L, t) \sim t^{1/4}$ with $\beta = 0.25$ and after a long time it saturates and reaches a steady state as $W(L, t) \sim L^{1/2}$ [1]. In (2+1) dimensions the surface width varies logarithmically with both t and L [1,5], with $\alpha = \beta = 0$. It should be noted that the case which includes surface diffusion is in contrast to that of the random deposition model. In the latter case there is no correlation between columns, and the height of the columns follows the Poisson distribution with $\beta = 0.5$ and undefined α, independent of dimension, while for the model with diffusion the correlation exists as a result of the effect of the surface diffusion.

In this case, i.e. the random deposition model with surface diffusion, the growth can be described by the Edwards–Wilkinson (EW) equation [6] which is

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

where the $v \nabla^2 h$ term tends to smooth the surface. The scaling arguments as well as the analytic solution of the EW equation give the following exponents:

$$\alpha = \frac{2 - d'}{2}, \quad \beta = \frac{2 - d'}{4}, \quad z = 2, \quad (4)$$

where $d' = d - 1$. It is indicated from the above equation that for $d = 2+1$, $\alpha = \beta = 0$.

In previous studies [7,8] we have shown that the model for two kind of particles, A and C, in (1+1) dimensions belongs to the EW universality class although there is a deviation for the calculated values of the exponents from those of the EW class. In this study, further results in (2+1) dimensions are reported. 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 dynamic scaling behaviour of the surface growth is studied with various system sizes and probabilities P as well as the morphological structure of the aggregates.

2. Growth model

In this model the particles, active particles A and non-active particles C, are allowed to fall randomly, one at a time, onto a growing surface and stick where they land or diffuse to another position depending on their types [8]. In general, a site is chosen randomly and then with a probability $1 - P$ (or P) a particle A (or a particle C) is deposited on the surface. The deposition occurs when the falling particle, whatever its type, meets a particle A on the surface. If the arriving particle is of type C, it is allowed to diffuse to a local minimum around the chosen site. On the other hand, if the incoming particle is of type A, it

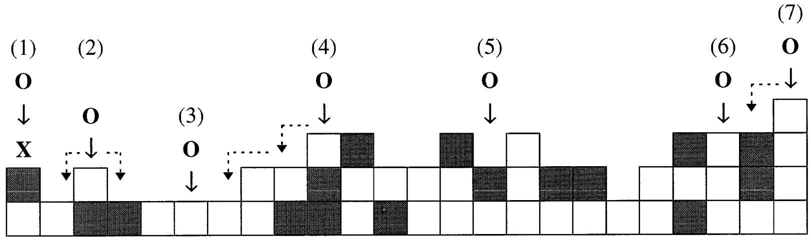

Fig. 1. The random deposition-like model of two kinds of particles. The white squares represent A particles and the grey squares denote C particles. The arrows indicate the paths of the deposited particles while the broken arrows show the paths which the particles diffuse along.

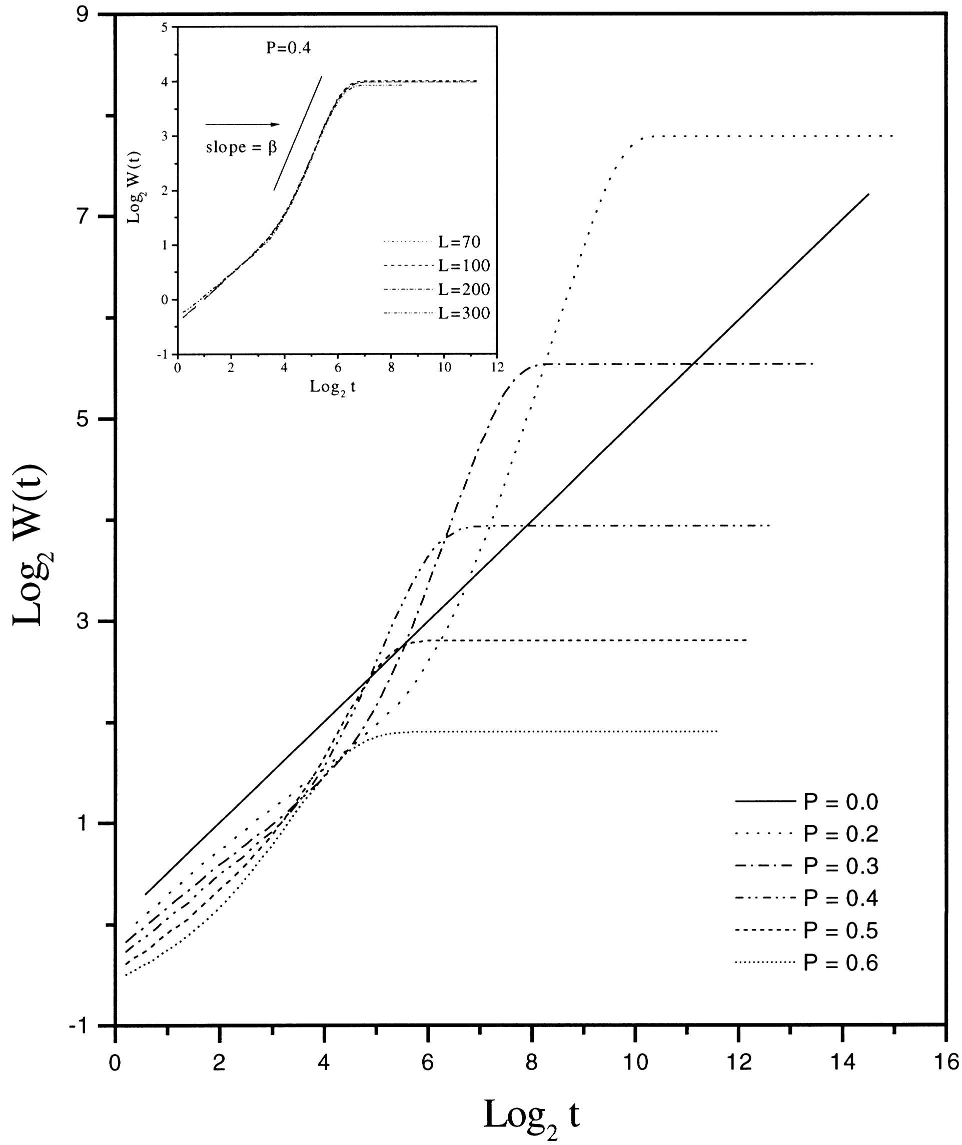

Fig. 2. $\log_2 W(t)$ versus $\log_2 t$ for a system of size $L=300$ and for different probabilities P. The inset shows how the exponent β is measured.

deposits where it lands. A cut of the aggregate is shown in Fig. 1, where A particles are depicted by white squares and C particles by grey squares. The deposition occurs according to the following rules. (a) If the incoming particle meets a particle A on top of the chosen site, and this site is higher than any of its surrounding sites, then it sticks to this site. If the deposited particle is of type C then it is allowed to diffuse along the broken paths to a site of minimal height around the chosen site (fallen particles 2, 4 and 7), noting that, in the case of fallen particle 2, the particle C will diffuse along any one of the equally probable descending paths. (b) If the incoming particle meets a particle

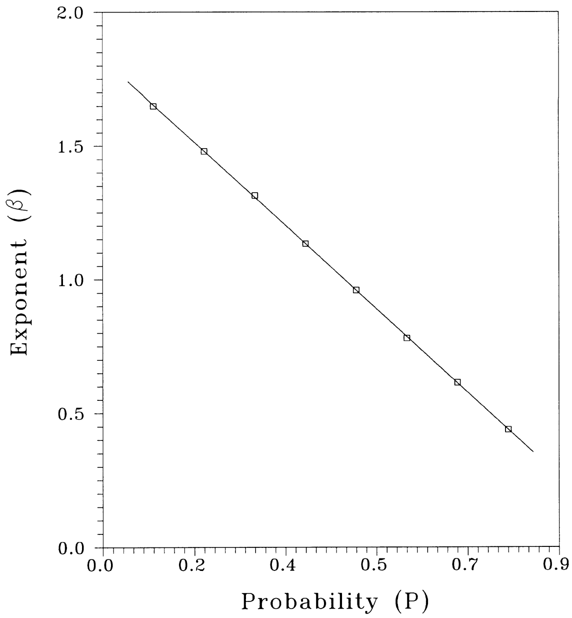

Fig. 3. The exponent β as a function of the probability P.

A on the top of the selected column that is equal in height to its neighbours, the particle sticks to that column regardless of its type (fallen particles 3 and 6). (c) If the selected column has a particle C on top of it and is lower than its neighbours, the deposition occurs only if one of the neighbouring sites has a particle A in a position higher than the chosen site by one step (fallen particle 5). (d) If the arriving particle meets a particle C on the top of the selected column, the deposition is excluded (fallen particle 1). The only case of deposition over a particle of type C is when a diffusion process ends in a local minimum which contains a particle C (fallen particles 2, 7) or process (c) occurs.

We have chosen this model since it may describe several physical processes. It is adequate for chemical reactions which take place on the growing surfaces of materials (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 to have a probability $1-P$, and the particle B a probability P. Thus, in this system, some of the surface sites continue to react while others do not. It may also represent the surface growth of a material with a low concentration of impurities. Particle C, which has fewer active bonds than particle A, plays the role of these impurities. Thirdly, it can model the deposition of two kinds of particle (one heavy and one light) with different attractive forces. Finally, the growth processes might be considered as a kind of percolation of the particles [9,10]. The deposition of particles A introduces connective bonds for the incoming particles A and C, while the deposited particle C prevents 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 non-active particle C.

For this model, the diffusion process for particle C is that this kind of particle is always deposited at a local minimum height. Such a type of diffusion has been used in many deposition models and it mimics the actual process that might happen during real growth [1]. Obviously, for $P=0$, the deposition mechanism of our model is just the same as in the random model (RD) [3], which is

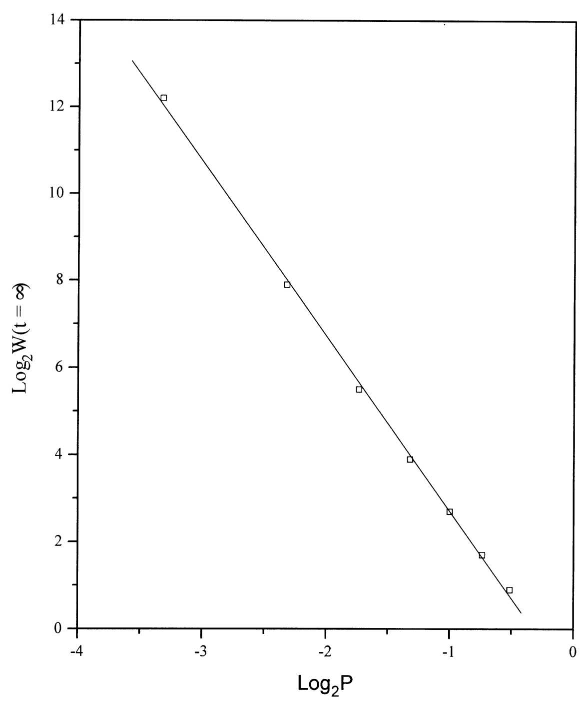

Fig. 4. $\log_2 W(t=\infty)$ versus $\log_2 P$.

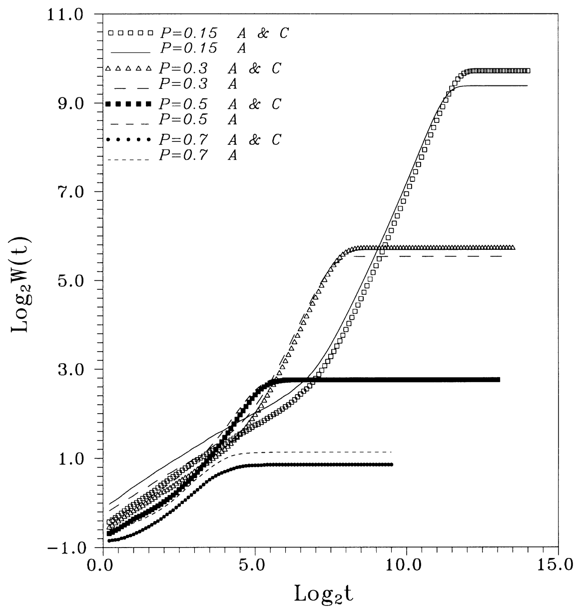

Fig. 5. $\log_2 W(t)$ versus $\log_2 t$ for when C only diffuses and for when both A and C diffuse.

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, they grow independently; however, the surface is rough. When $P \neq 0$, once a particle C is deposited on a column, its growth will depend strongly on the local structure. This introduces correlations between the different columns. Thus in this case some of the surface sites continue to grow while some sites do not. Diffusion is introduced only for particles C since they have fewer bonds interacting with other particles and they can move more freely to a place with lower height.

3. Dynamical scaling behaviour

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

Fig. 2 shows a plot of the surface width W as a function of time t (number of deposited layers) for different values of the probability P. As shown in this figure, when $P=0$ there are no correlations between the columns, and the width of the surface grows with time having an exponent equal to 0.5. For $P \neq 0$ the scaling behaviour is changed and the growth of the aggregate is divided into three stages. First at an early time, non-fixed time intervals from $\log_2 t=6.5$ for $P=0.2$ to $\log_2 t=1.5$ for $P=0.6$, the surface width grows with time as $W \sim t^{1/2}$ with little deviation from this behaviour for $P>0.5$. Later the surface width grows as $t^{\beta(P)}$; it is in this interval that we measure the exponent β as indicated in the inset of Fig. 2, which shows a plot of the saturation width as a function of time for a value of $P=0.3$. This inset reveals that the surface width is independent of the system size [7]. We have carried out simulations for different values of P and found the same features. We argue that this is due either to finite-size scaling or to multiscaling and lack of self-affinity associated with instability [11]. Finally the surface width saturates and reaches a constant value. It is clear from Fig. 2 that a system instability occurs [12] since for $P<0.5$ there exist two different time intervals representing two different regimes. However, during the early time the surface grows with an exponent approximately equal to 0.5, which means growth with no or with weak correlation. Therefore, we measure the exponent β in the intermediate interval of time [7]. As P increases, the early time interval decreases and reaches to values less than $\log_2 t=2$ for $P \leq 0.5$. So, this small time interval can be considered as a transient [5] and stable growth occurs. Fig. 3 supports the above indications, which shows the exponent β as function of P. It is clear from this figure that $\beta(P)>1$ for $P>0.5$ pointing to an instability, while $\beta(P)<1$ for $P \geq 0.5$ which means a system stability. Fig. 4 shows the surface width at saturation versus the probability P for $L=300$. From this figure the surface width is scaled with the probability; $W(t=\infty) \sim P^{-\gamma}$ with $\gamma=3.74$.

The above results are, in fact, rather surprising. It is true that the mechanism of growth for the random deposition model with surface diffusion is described by the EW theory where $\beta=0$ in $(2+1)$ dimensions. However, the simulation in our case shows that the surface width grows with time

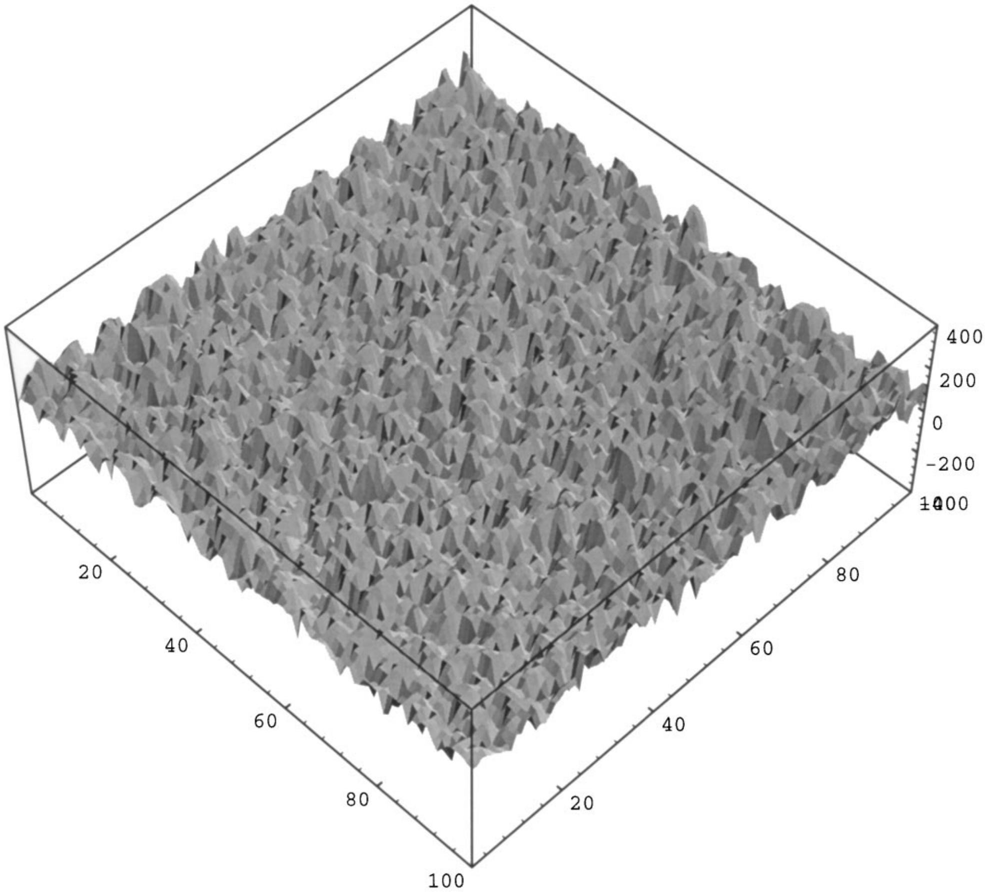

Fig. 6. (a) Surface plot for $P=0.3$; (b) density plot for $P=0.3$.

according to an exponent $\beta(P)$. The values of $\beta(P)>1$ for $P<0.5$ suggest an instability of the system where a surface with pillars and groves are formed.

Since diffusion of particle A is not included in our model and the results may be due to the diffusion of only particles C, we have performed simulations when the diffusion is allowed for both particles A and C. Fig. 5 shows the surface width versus time for different probabilities. As indicated in the figure for $P<0.5$, the surface widths in the case when only C diffuses are lower than those when both A and C diffuse. The reverse feature is observed for $P>0.5$. When $P=0.5$ the surface widths are the same in both cases. Away from that, no change in the behaviour can be seen. This indicates that this anomalous kinetics of growth is mainly due to the type of interactions between particles and not to the dynamics of the diffusion of different particles.

4. Morphology

In this section, we introduce the morphological structure in order to interpret the kinetics. Fig. 6a shows three-dimensional plots of the surface for $P=0.3$. The density plot of corresponding to the given surfaces in Fig. 6a is presented in Fig. 6b, where black represents the lowest height and white is the highest one. From the surface shape and its corresponding density plot, the variation between column heights is large, which reveals the presence of an unstable growth morphology where pillars

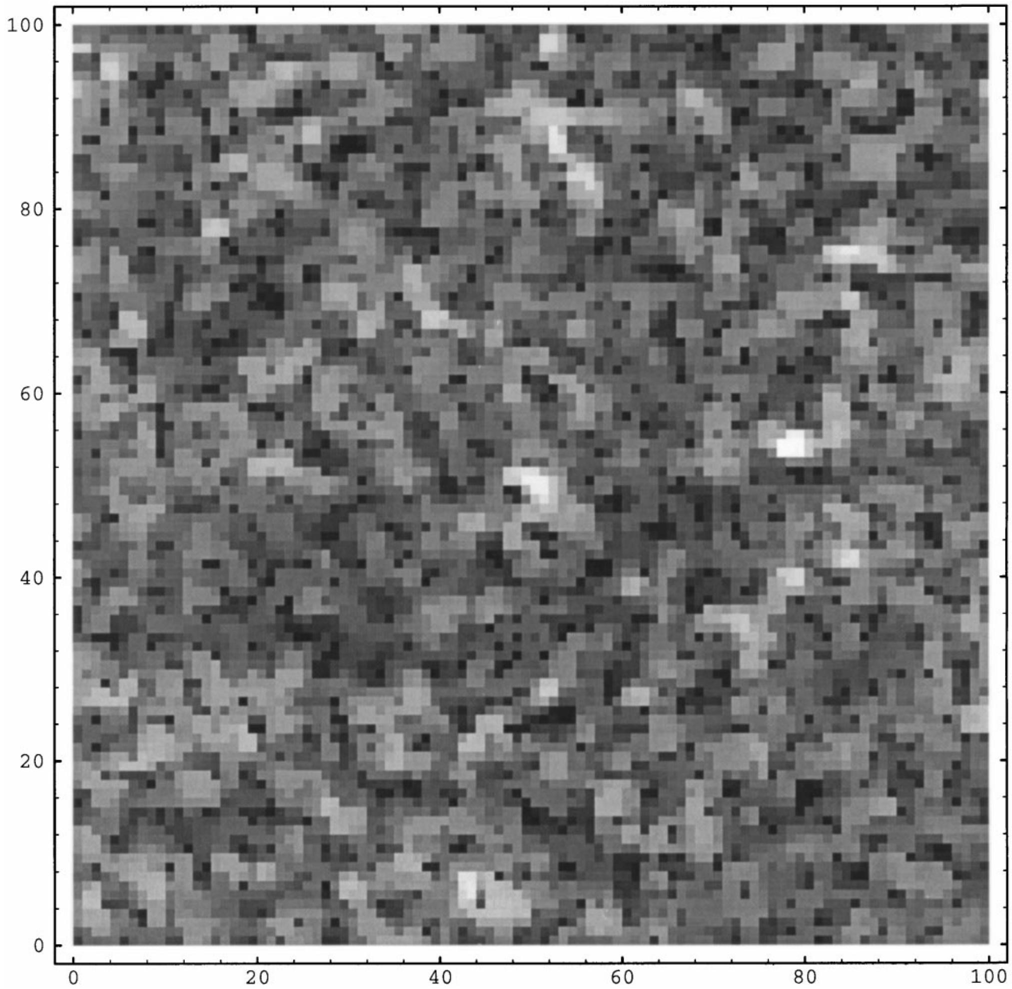

Fig. 6. (*continued*)

and grooves are formed on the surface. The instability is suppressed as P increases and then vanishes when P exceeds 0.5 where the exponent $\beta(P)<1$.

Fig. 7 shows a cross-sectional view of the final stage of the aggregate and the distribution of the two kinds of particles throughout part of the bulk for $P=0.3$. From the plot, it can be seen that the growth of a column stops (is quenched) when it has a particle C on top of it as well on the top of its neighbours (four neighbours higher by one step). For $P<0.5$, the probability of being a particle C is small and few columns have been halted very early while the others grow. This causes a large height fluctuation along the surface which leads to the formation of high pillars and deep grooves that increase the surface gradient.

The existence of such grooves is the reason that $\beta(P)$ is greater than unity for $P\leq 0.5$. For $P>0.5$, where $\beta(P)<1$ the chance that more columns will be blocked earlier during the growth becomes high, since the probability of being a particle C is high and hence the growing sites cannot be too much higher than the blocked sites. So the difference between column heights becomes small, leading to the disappearance of pillars and grooves from the surface and stable growth. It also causes earlier

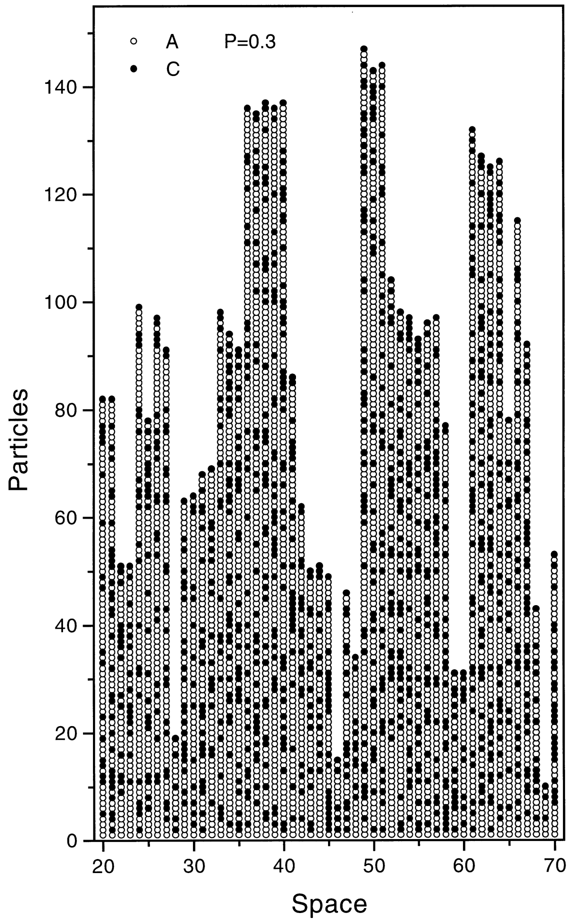

Fig. 7. Cross-sectional view of the final part of the aggregate for $P=0.3$.

saturation of the surface than in those cases where P is low. At saturation, the surface as a whole is covered with particles C.

Qualitatively, the above discussion can be interpreted in terms of directed percolation. Blocked columns try to stop the growth while the interface advances on other parts. In other words, some parts of the interface are pinned. After some time, as a result of the diffusion of the non-active particles, the number of the blocked columns increases. Thus the resistance against the interface to advance increases and its velocity is greatly affected. The interface is pinned when it is completely covered by particles C. At this moment the non-active particles connect themselves to form a

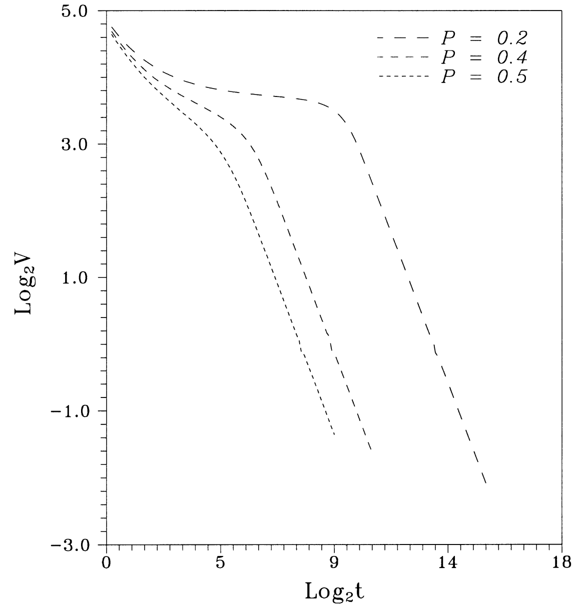

Fig. 8. The interface velocity versus time for different values of P.

large inert cluster which blocks the connection between the active particles. Fig. 8 shows the interface velocity versus time for different values of P. It is clearly seen from this figure that the velocity decreases and then finally reaches zero when the line indicated on the graph is terminated.

From the above discussion, the situation on the surface is as follows. During the growth there exist few clusters of particles C of small sizes distributed over the surface. As time increases, these clusters spread out until they cover all the surface sites. Fig. 9 shows the surface view at different values of time, $\log_2 t=5.5$ and $\log_2 t=8$ for $P=0.3$, respectively. The spreading of clusters of particles C (non-active clusters) suggests a non-locality in the growth where the flux of the particles is captured by some sites. This also leads to high fluctuations in height and unstable growth morphology as indicated by the value of $\beta>1$.

5. Discussion and conclusion

For the random deposition-like model, we have implemented a physically realistic process for non-

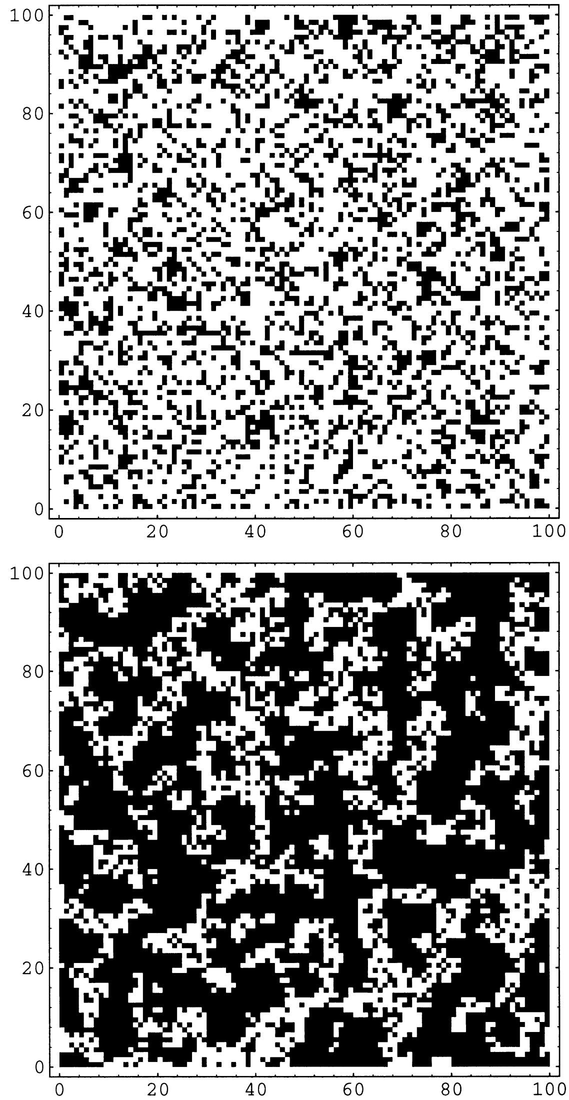

Fig. 9. Snapshots of the distribution of particles on the surface for $P=0.3$: (a) $\log_2 t=5.5$ and (b) $\log_2 t=8$.

active particles C to diffuse. Immediately after deposition, the particle C moves via a random walk along the surface. It stops when it reaches either a local minimum or when it has moved l_d steps on the surface. In other words, there is a diffusion length for particle C. In our work, this length is limited to 20 lattice spaces, which is rather large and may describe the experimental situation at high temperatures. For low probability P, almost all the diffusion stops within a distance less than l_d since the morphological structure is locally rough. For high values of P the diffusion steps are large and may reach the value of l_d. We also carried out several runs for different values of l_d larger and smaller than 20, for different possibilities, and we found that the scaling properties of the surface are basically the same.

Unstable growth morphology occurs in non-local growth models when smoothing by surface diffusion competes with the instability as well as in models for diffusion bias where an uphill current occurs owing to formation of barriers (see discussions in Ref. [5], chapters 19 and 20). Although the mechanisms that induce the instability are different in the above-mentioned cases from those in our case, we can qualitatively relate the instability in our model to that in the other cases. On the one hand the non-locality is caused by the formation of clusters of particles C which isolate the clusters of the active particles A. Therefore, zones of particles A continue growing while other of type C stop. Thus, large fluctuations in height result, which influence the instability. As P increases, the diffusion competes with this instability because of the presence of more particles C. On the other hand, for low values of P, the diffusion of particles C is limited since columns that contain particles A grow more than those with C which give rise to barriers on the surface. So, the morphology of the surface is dominated by high pillars and deep groves. This means that step slopes are generated on the surface which increase as more deposition occurs and finally instability appears.

All of the above discussion as well as the finite size scaling prompt us to argue that the surface may not be self-affine or that a multiscaling is present [12,11]. However, in order to clarify this argument and to determine which universality class our model belongs to, a further detailed study is required.

In conclusion, we have proposed a growth kinetics of two kinds of particles A and C in (2+1) dimensions for the random deposition-like model. The scaling results show the existence of the exponent $\beta(P)$ as well as an unstable growth morphology for $P<0.5$. For $P\geq 0.5$ the kinetics and the morphological study denote that the instability ceases.

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