# Growth kinetics and morphology of a ballistic deposition model that incorporates surface diffusion for two species

Hassan F. El-Nashar
*Department of Physics, Faculty of Science, Ain Shams University, Cairo 11566, Egypt*

Hilda A. Cerdeira
*The Abdus Salam International Centre for Theoretical Physics, P.O. Box 586, 34100 Trieste, Italy*
(Received 31 August 1998; revised manuscript received 12 January 1999)

We introduce a ballistic deposition model for two kinds of particles (active and inactive) in $(2+1)$ dimensions upon introducing surface diffusion for the inactive particles. A morphological structural transition is found as the probability of being the inactive particle increases. This transition is well defined by the change in the behavior of the surface width when it is plotted as a function of time and probability. The exponents $\alpha$ and $\beta$ calculated for different values of probability show the same behavior. The presence of both types of particles gives rise to three different processes that control the growing surface: overhanging, nonlocal growth, and diffusion. It finally leads to a morphological structural transition where the universality changes away from that of Kardar, Parisi, and Zhang, in $(2+1)$ dimensions, but not into that of Edwards and Wilkinson. [S1063-651X(99)05607-X]

PACS number(s): 05.40.−a, 05.70.Ln, 68.10.Jy, 68.35.Ct

## I. INTRODUCTION

The growth of surfaces and interfaces has recently attracted great interest motivated by technological applications. Most rough surfaces are formed under conditions that are far from equilibrium. Therefore, the study of such phenomena has a relevant importance in understanding nonequilibrium statistical mechanics at the fundamental level. Simple models have played a major role in this understanding by studying two important aspects, kinetics and morphology. Kinetics helps to understand how surfaces evolve with time while morphology provides a clear interpretation of the growth kinetics [1–3].

It is well known that a stochastically growing surface exhibits scaling behavior and evolves to a steady state without a characteristic time or length scale. Therefore, starting with an initially flat substrate, defining the surface width $W(L,t)$ by

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

where $L$ is the system size, $h(r,t)$ is the height of the surface at position $r$ and time $t$, $\overline{h(t)}$ is the average height at time $t$, and $d-1$ is the substrate dimension, the scaling law [4] is given by

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

The roughness exponent $\alpha$ and the growth exponent $\beta$ characterize the dynamical scaling behavior. The function $f(x)$ scales as $f(x)=x^{\beta}$ for $x\ll 1$ and $f(x)=\text{const}$ for $x\gg 1$. This scaling behavior has been studied in various systems and models and has been argued to be universal [1–3,5].

Among the models used to represent the growth of rough surfaces, a well-studied example is the ballistic deposition (BD) model. Here, particles rain down vertically onto a $(d-1)$-dimensional substrate and aggregate upon first contact [6], giving rise to a rather interesting structure: the surface is a self-affine fractal although the bulk, which is filled of voids inside, is compact [3]. One of the successful theoretical approaches to describe the BD model is that of Kardar-Parisi-Zhang (KPZ) equation [7],

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

which is a nonlinear equation for the local growth of the profile $h(r,t)$ of a moving interface about a $(d-1)$-dimensional flat substrate. However, although the BD model captures the essential features of processes such as vapor deposition, it does not provide an adequate representation of diffusion on the surface. Such processes can be found in growth where the newly arriving particle diffuses to a local minimum along the surface of the deposited material. Surface diffusion leads to surface relaxation which tends to smooth the surface [1]. Therefore, when a surface diffusion process is introduced, the linear term $\nabla^2 h$ representing diffusion will compete with the nonlinear term $(\nabla h)^2$, which symbolizes the lateral sedimentation in the KPZ equation. As diffusion becomes the dominant process, the linear term wins and the universality will be changed [8] to the Edwards-Wilkinson (EW) universality [9], which is described by the equation

$$\frac{\partial h}{\partial t}=\nu\nabla^2 h+\eta(r,t). \tag{4}$$

In this case voids are no longer formed inside the bulk as a result of the reconstruction trend during the growth [1]. Also in this case for $(2+1)$-dimensional growth the exponents $\alpha=\beta=0$ due to the logarithmic variation of the surface width with both time and system size, respectively.

Most previous studies have dealt with the surface growth of one type of particles [1–3,5]. Generally, in the growth of

 

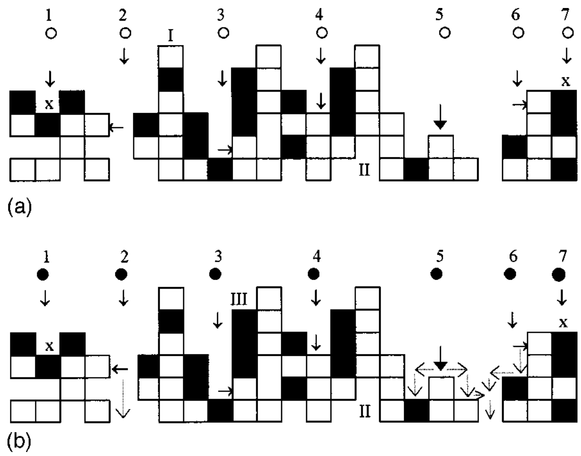


FIG. 1. A cross sectional piece of the aggregate. White squares stand for particles *A* and dark squares symbolize particles *C*. (a) The empty circles denote the deposited particles of type *A*. The deposition is indicated by the arrows. (b) The full circles represent particles of type *C*. The deposition is indicated by arrows. The process of diffusion is represented by fallen particles 5 and 6.

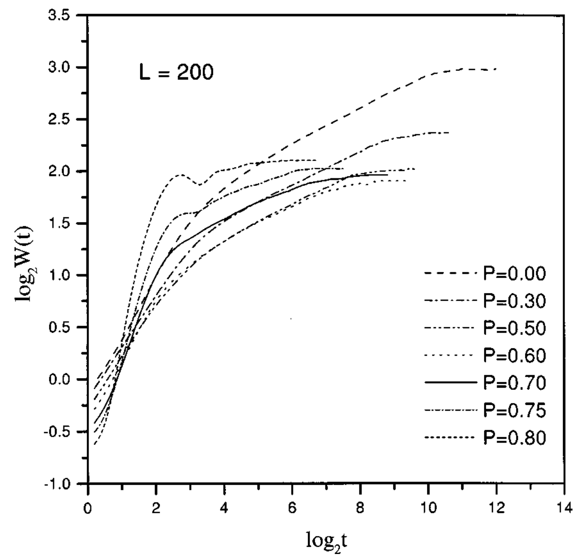


FIG. 2. Log-log plot of the surface width versus time for different values of *P* at fixed size $L=200$.

real materials one should take into consideration that different kinds of particles are deposited. Thus, in the growing system, there may exist different kinds of interactions for different particles, which in turn yields a different kinetics of growth associated with a change in the morphological structure of the aggregate. Pelligrini and Jullien (PJ) [10,11] described a surface growth according to a model with two kinds of particles, sticky and sliding, where both are active. This model interpolates between a diffusive model which incorporates surface diffusion and the usual ballistic deposition model. They used a parameter *c* to control the process of diffusion on the surface. When $c=0$ their model is similar to that of Family [12], i.e., a model with surface reconstruction, while, when $c=1$, it is equivalent to the plain ballistic model. However, they do not present the kinetic study and how the surface evolves with time to a steady state. In previous reports [13–15], we have used a BD model for two kinds of particles (active and inactive) but without including diffusion on the surface and found a morphological structural transition as the probability of being an inactive particle increases. Such transition is attributed to the presence of both types of particles and the tendency to form more vacancies inside the bulk of the aggregate where overhanging becomes dominant. At the same time there exists a nonlocal growth due to the formation of particle *C* clusters on the surface that do not allow other particles to stick over them.

In this work, we present a BD model for two kinds of particles; one of them is active with probability $1-P$ and the other inactive with probability *P*, with a surface diffusion towards a local minimum for the inactive particles. We use the probability *P* as a continuously tunable parameter to control the system. We depict the growth kinetics in $(2+1)$ dimensions as well as the morphological structure in order to interpret the results which have been obtained. We will show that such diffusion processes will not change the universality class from KPZ to EW. The appearance of different types of particles may strengthen the lateral sedimentation which in turn provokes formation of voids under the surface as well as nonlocal growth by virtue of the constitution of inert clusters of particles *C* on the surface: a competition between the diffusion process on the surface and overhanging and nonlocal growth may happen. Although the diffusion may suppress the effect of nonlocal growth, it will not completely cancel that of overhanging. Therefore, the Laplacian term $\nabla^2 h$ will not overcome totally the nonlinear term $(\nabla h)^2$ in Eq. (3), which will not reduce to Eq. (2).

The presentation of this paper is as follows. In Sec. II, the model and the physical motivations are presented. In Sec. III, the dynamical scaling behavior and the morphology are discussed. Finally, a conclusion is given in the last section.

## II. DEPOSITION MODEL

We consider a model composed of two kinds of particles, *A* and *C*, which fall on a square substrate of size $L^2$, with probabilities $1-P$ and *P*, respectively. Particle *A* is active,

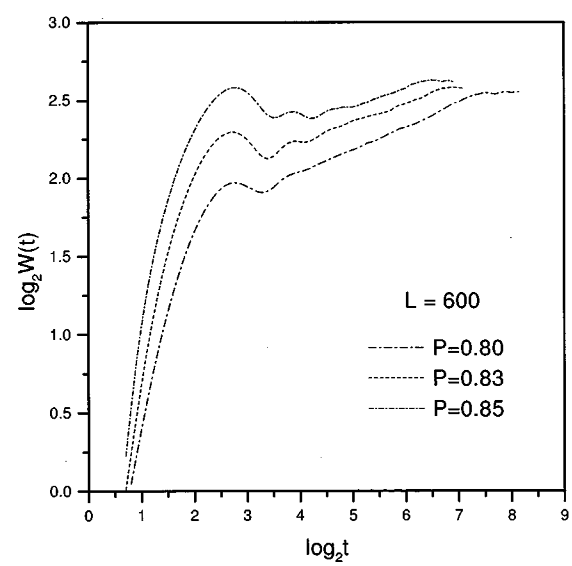


FIG. 3. Surface width as function of time for $P>0.8$ when $L=600$.

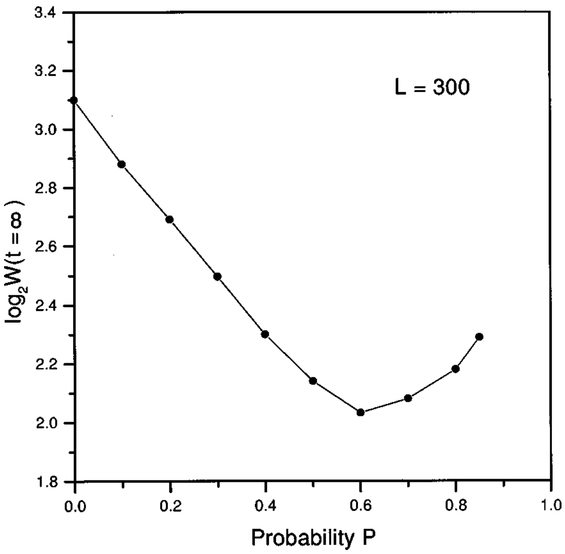


FIG. 4. Saturated surface width versus the probability when $L=300$. The connected lines are drawn for convenience.

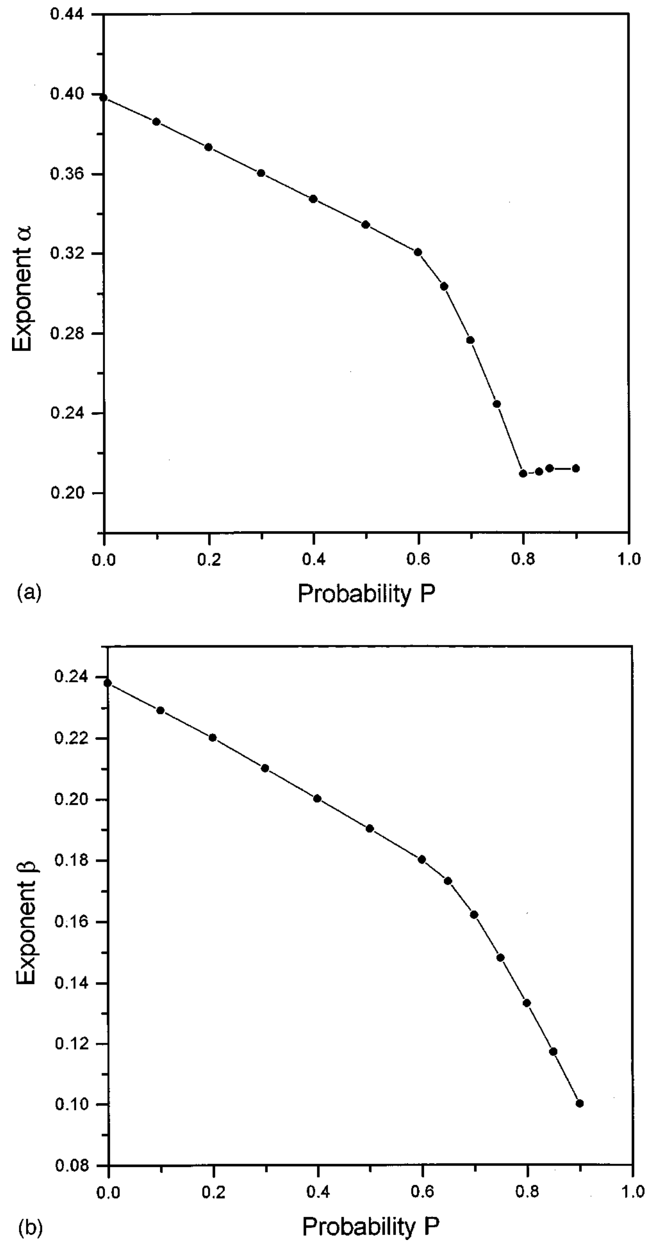


FIG. 5. Probability versus (a) the exponent $\alpha$ and (b) the exponent $\beta$. The lines connecting points in each curve are drawn for convenience.

while particle $C$ is inactive; the meaning of active and inactive will become clear after the description of the process.

The model we propose is appropriate to describe chemical reactions which take place on the growing surface of materials. For instance, 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 $P$. 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. It also represents the surface growth of a material with low concentration of impurities. These impurities are represented by particle $C$ which has fewer active bonds than particle $A$. Further, it describes the deposition of two kinds of particles (one heavy and one light) with different attractive forces.

The growth process, which consists of particles falling randomly straight down one at a time onto a growing surface, is as follows: at first a column is selected at random and then a particle $A$ (or particle $C$) is deposited on the surface of the aggregate with a probability $1-P$ (or $P$). A cross section of the aggregate is shown in Figs. 1(a) and 1(b). The white squares represent the aggregated particles of type $A$ and dark squares represent those of type $C$. Circles, which account for both types $A$ (empty) and $C$ (full), denote the incoming particles. The path of the fallen particle is shown by the arrows. The deposition of particles of type $A$ occurs according to the following processes depicted in Fig. 1(a): particle $A$ will stick to the first particle $A$ that it meets, either at the top of the chosen column (particles 4 and 5) or sideways (particles 2, 3, and 6); on the other hand, if no particle $A$ is found the incoming particle will be discarded (particles 1 and 7). When the incoming particle is of type $C$ [process shown in Fig. 1(b)], it does not stick to the top of the chosen column if the latter is higher than the neighboring columns: it diffuses if it meets a particle $A$ (particle 5) or it is discarded if it finds a particle $C$ (particle 7); on the other hand, if the chosen column is lower than its neighbors and the highest neighbor contains particle $A$, the particle will diffuse if there is at least one neighboring column lower than the chosen one (particles 6) or it will diffuse downward (particle 2); when all the surrounding columns are higher than the chosen one, the incoming particle will stick on top of it if it finds a particle $A$ either at the top (particle 4) or sideways (particles 3), otherwise the particle will be discarded (particles 1 and 7). Therefore, the only process of deposition of particles over inactive ones (type $C$) happens when through lateral sedimentation (fallen particle 3) or diffusion (fallen particle 5) they stick to a particle $A$. Otherwise, the particle should be discarded. Notice that a process of type I, in Fig. 1(a), where a particle $A$ has deposited on top of a $C$, can happen because in $(2+1)$ dimensions there are four neighbors and the particle adheres to a side of any of those neighbors. Also a process of type II occurs due to overhanging to any one of the four neighbors

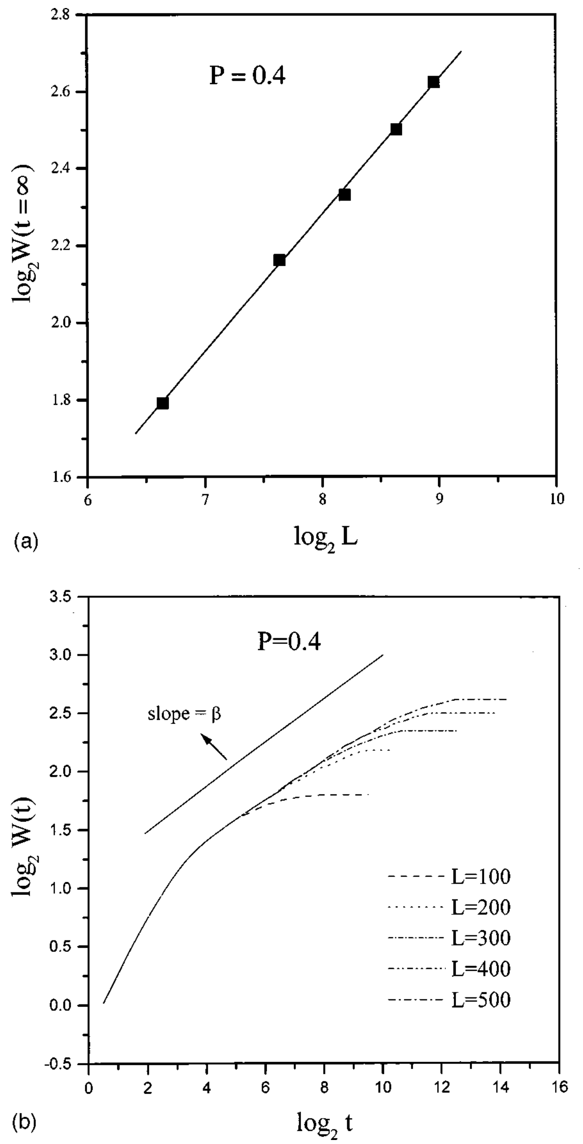


FIG. 6. (a) Log-log plot of the lattice size and the saturated surface width when $P=0.4$; the calculated exponent is $\alpha=0.35 \pm 0.007$. (b) Log-log plot of the surface width versus time for different sizes when $P=0.4$; the calculated exponent is $\beta=0.19 \pm 0.01$.

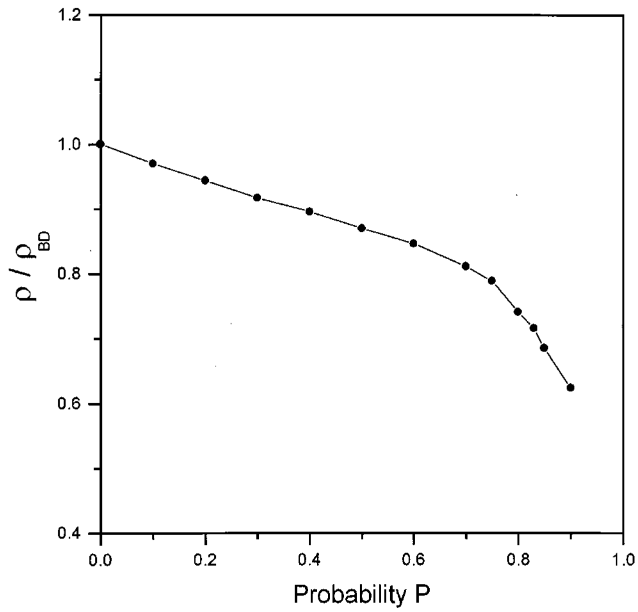


FIG. 7. Bulk density measured relative to that of BD versus the probability. The lines between points are drawn for convenience.

higher than the chosen site. A process of type III arises since particles *C* always diffuse to the local minimum on the surface and maybe this site is located at the edge of the area of local diffusion.

Finally, the surface growth processes of the particles on the aggregation might be considered as a kind of percolation of the particles [16]. 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* to stick to it. The surface keeps growing as long as the surface sites are not entirely covered by the inactive particle *C*.

### III. RESULTS

We performed simulations for this model on a square lattice with $d=3$. The aggregation occurs in the *Z* direction with boundary conditions in the *X* and *Y* directions. Statistical average is obtained over 500 independent simulations for each parameter. All simulations have been carried out for system size $L>100$ to go beyond the limit of size dependence.

Figure 2 shows a log-log plot of the surface width *W* as a function of time *t* (number of deposited particles) for different values of the deposition probability *P* and fixed system size $L=200$. It is seen from this figure that the surface width increases fast and finally saturates to a fixed value after experiencing a slowdown. For $P=0$ the curve represents the usual BD model for only one kind of particles [13,15]. The scaling result for the exponent $\beta$ is the same as for the BD model, that is, $\beta=0.238\pm 0.005$ [5]. For values of $P\neq 0$, the surface width decreases as the probability increases and the saturation state is reached early. However, for $P>0.6$, the surface width increases again and the system saturates faster. It also appears that for $P\geqslant 0.75$ there is a reduction in the surface width which increases in depth as the probability increases. We cannot perform simulations for $P>0.9$ due to the disappearance of bonds between particles along the surface. In order to be sure that such decrease in the surface width does not depend on the system size, we performed simulations up to $L=600$. The results are shown in Fig. 3, which reveals clearly the behavior of the surface width as the time increases. The figure also shows for $P>0.8$ a small oscillation in the surface width which disappears for long times and $W(t)$ changes as $t^{\beta}$. It should be noted that in the case of $P>0$, up to the limit of our calculations in time, we have not found a steady state where the surface finishes completely covered with inactive particles and stops growing altogether. We conjecture that this is due to the presence of the active particles *A* which allow the incoming particles to stick laterally or over them. In addition, due to diffusion, particles of type *A* are either left uncovered or their sides are free. In Fig. 4, we plot the saturated surface width versus the probability for a system size $L=300$. We see that the saturated surface width varying with the probability *P* shows a non-

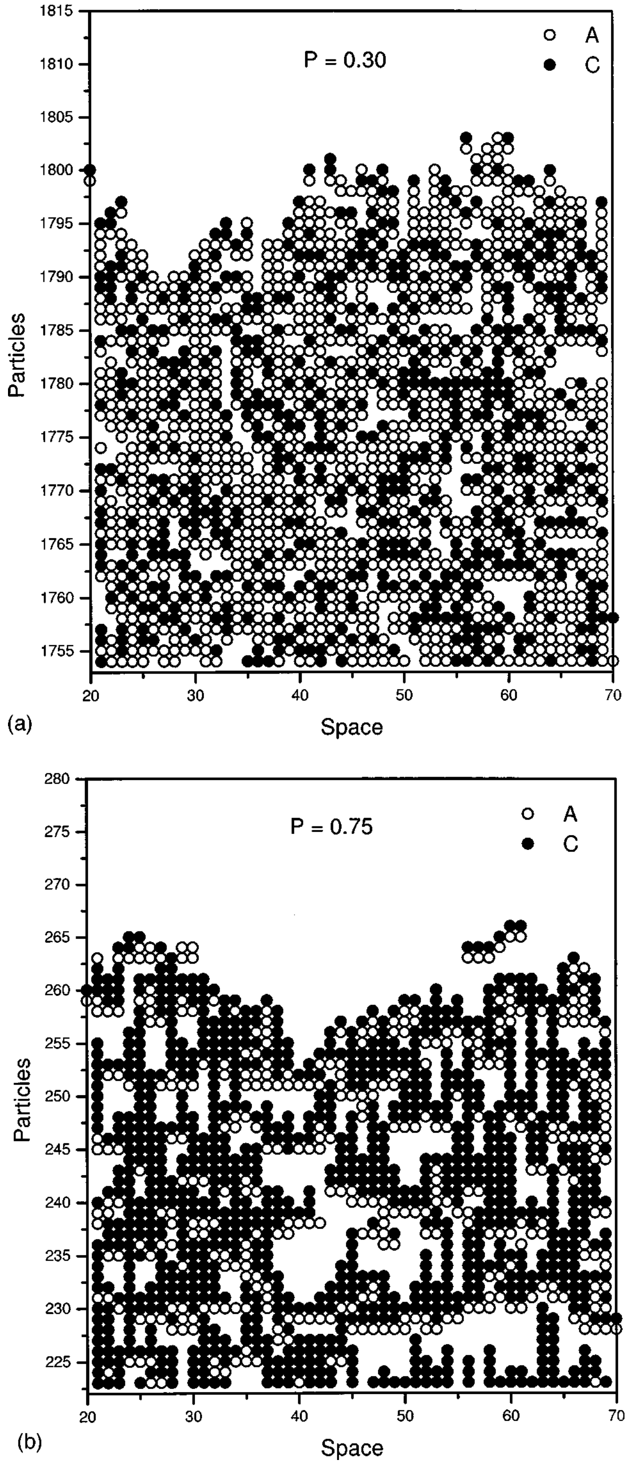


FIG. 8. Cross sectional view of the final part of the aggregate for (a) $P=0.3$ and (b) $P=0.75$.

monotonic relationship, that is, $W(t=\infty)$ first decreases and then increases as the probability $P$ increases, with a minimum around $P=0.6$. We have plotted the exponents $\alpha$ and $\beta$ as a function of the probability $P$ in Fig. 5. We find that $\alpha$ changes linearly upon increasing probability for $P\leqslant 0.6$. It decreases rapidly until $P=0.8$, after that it fluctuates around a fixed value as shown in Fig. 5(a). Figure 5(b) reveals the same feature for the exponent $\beta$ where it decreases linearly as a function of the probability for $P\leqslant 0.6$ and then suffers a rapid decrease until it becomes 0.1 for $P=0.9$. Figure 6

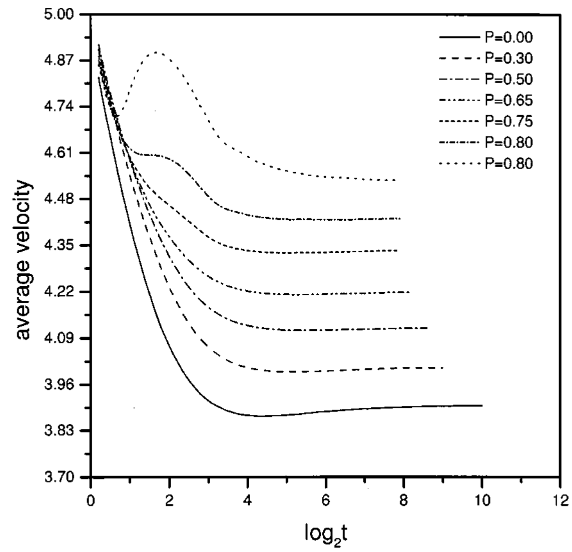


FIG. 9. Average velocity as a function of time for different values of $P$.

shows how we obtained the exponents $\alpha$ and $\beta$. The calculated exponents are (a) $\alpha=0.35\pm0.007$ and (b) $\beta=0.19\pm0.01$ for $P=0.40$.

The results found above point clearly to a change in the morphological structure of the surface as $P$ increases. It is obvious from the behavior of the surface width and the values of the exponent $\alpha$ and $\beta$ that for $P=0$, the morphology is similar to that of the BD model [5]. Such behavior is changed as the value of $P$ increases. The results suggest that surface diffusion will not be the only process that controls the growth. In fact, the existence of two different types of particles allows overhanging. Also, the development of clusters of particles $C$ on the surface leads to a nonlocal growth. Therefore, diffusive particles tend to reconstruct the surface and suppress the effect of the nonlocality. However, diffusion cannot entirely remove the overhanging and the existence of voids. This means that the term $\nabla^2 h$ does not manage exclusively to suppress the nonlinear term $(\boldsymbol{\nabla} h)^2$ and the transition will not be from Kardar-Parisi-Zhang universality to that of Edwards and Wilkinson. The result of the competition between both terms influences the surface width to grow as $W(t)\sim t^{\beta}$ even when the probability of being a diffusive particle $C$ is high. Alternatively, it means that in addition to surface diffusion, overhanging processes and formation of voids occur. This led us to investigate the compactness of the bulk. Figure 7 shows the probability versus the density of the aggregate $\rho=N/\langle h\rangle L^2$ which is measured relative to the density of the usual BD model, where $N$ is the number of columns of the whole aggregate, $\langle h\rangle$ is the average height, and $L^2$ is the system size. It is obvious from this figure that the density of the bulk decreases as $P$ increases. This reflects clearly the occurrence of the overhanging process during the growth which increases as $P$ increases. Figure 8 reveals the constitution of empty spaces under the surface which expand as the value of $P$ rises. In fact, as shown in previous works [13–15], overhanging enlarges the local gradient of the surface and enhances the process by which particles stick perpendicularly to the local gradient, thus increasing the nonlinear growth. Furthermore, the presence of inactive particles over the surface induces the

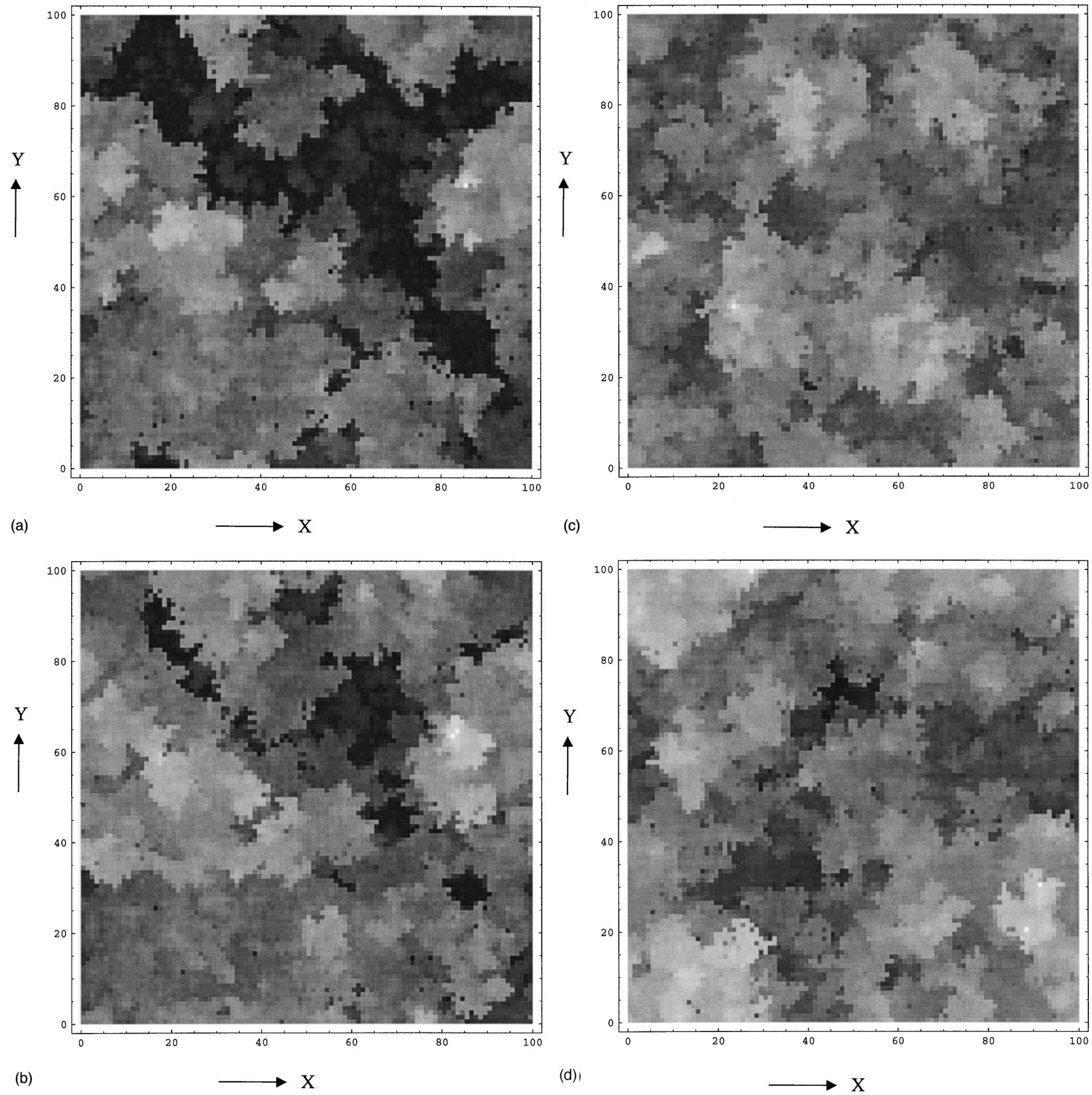


FIG. 10. View of the surface from the top as density plots for column heights. (a) at $\log_2 t=2$, (b) at $\log_2 t=3$, (c) at $\log_2 t=3.7$, and (d) at $\log_2 t=8$.

constitution of wide and deep grooves on the surface leading to the flux of particles to be captured by some sites. Thus, the surface width grows with time, having a large value of $\beta$. However, in the present case, overhanging and nonlocality are not the governing processes since at the same time there is surface diffusion. The latter diminishes the increase of the surface gradient originated by overhanging although it does not completely overcome the creation of vacancies under the surface. Also, diffusive particles remove the effect of nonlocality when they move over the surface to the local minimum. So, the surface width finally grows with a certain value of $\beta$, which is neither high nor zero, and it does not vary logarithmically with $t$ and $L$ as in the models with surface reconstruction in $(2+1)$ dimensions.

We return to the strange behavior in the kinetics that we mentioned previously. It is clear from Figs. 2 and 3 that there is a dip in the surface width as well as an oscillation as it varies with time. We argue that this behavior is due to the competition between overhanging and surface reconstruction processes. In Fig. 9 we plot the average velocity as a function of time. It is seen from this figure that for small values of $P$ the average velocity decreases with time until it finally reaches a constant value. For $P \geqslant 0.75$ a change in this behavior starts to occur. There exists a decrease for very small values of $t$, we omit it since it is considered a transient [5], then the average velocity increases, stabilizes for a short while, and then decreases until it reaches a constant value. This first increase suggests that at such time the growth is dominated by overhanging and nonlocality which leads to a rapid increase in surface width and to an early saturation. Then, diffusion becomes relevant and more effective in playing its role. However, over some period of time there exists a struggle between overhanging and nonlocality, and diffusion which causes this oscillation of the surface width. Finally, a balance between different processes occurs and the surface width grows as $W(t) \sim t^{\beta}$. This argument is sustained by Fig. 10, which shows the topography of the surface as a density plot of column heights at different stages of growth (white for the highest and dark for the lowest). Figure 10(a) shows a large variation between column heights which is attributed to the increment in the local surface gradient as a result of overhanging. The step slopes on the surface due to nonlocality can also be seen. To this moment surface diffusion has not produced a great effect to reduce such a function. This produces a fast growth rate. As time increases, surface diffusion takes over and the grooves disappear in view of the reconstruction. Figures 10(b) and 10(c) show this behavior while Fig. 10(d) shows the surface at very large time when the surface becomes rough but without large fluctuations in height as is predicted from the small value of $\beta$.

It is shown from Fig. 9 that the average velocity of the interface at saturation increases with $P$. When $P$ increases, more voids are created under the surface (see Fig. 8), which raises the interface velocity [5]. Also, overhanging magnifies the lateral spreading of the surface [15,17], which expands the lateral correlation length, reaching the value of $L$ faster; hence the surface width saturates earlier. However, for $P > 0.6$, the surface width saturates earlier in time with higher values. This is ascribed to the evolution of more voids at the early stage in addition to the nonlocality (see Fig. 10) where the interface is driven to grow with high velocity towards saturation at a fast rate [14,15]. Nevertheless, when surface diffusion becomes important, it overcomes the consequence of nonlocality and reduces the local surface gradient with respect to overhanging but not to void production. Consequently, the interface is driven to grow with small value of the growth exponent but with higher velocity and early saturation.

## IV. CONCLUSION

We have proposed a BD model for two species where a surface diffusion process is introduced. We have studied the kinetics and morphology of the surface growth for different probabilities of the species. We found that upon increasing the probability $P$, the surface width reduces and saturates faster until $P = 0.6$. After this value the surface width increases and saturates earlier with time. The measured values of the exponents $\alpha$ and $\beta$ change also for different values of $P$. However, as the diffusion process over the surface becomes dominant, the values of the exponents do not tend to the values of the Edwards-Wilkinson universality class, in contrast to the work of Pelligrini and Jullien [10,11]. They used a ballistic model for two kinds of particles when both of them are active. Their model stands between a plain ballistic model and a full surface reconstruction model and they found a change from the Kardar-Parisi-Zhang universality to Edwards-Wilkinson universality. We attribute the difference in our case to the behavior of the two types of particles which allow overhanging to endure. Furthermore, the inactive particles form clusters over the surface which promote the nonlocal growth. Overhanging and nonlocality try to enhance the surface gradient and height fluctuations, which, at the same time, are eliminated by diffusion.

## ACKNOWLEDGMENTS

H.F.E. would like to thank the Abdus Salam International Center for Theoretical Physics (ICTP) for hospitality during this work. Also, he would like to thank Professor M. Shalaby for his encouragement. H.A.C. acknowledges support from the Istituto Nazionale de Fisica Nucleare (INFN).

[1] F. Family and T. Vicsek, *Dynamics of Fractal Surfaces* (World Scientific, Singapore, 1990).
[2] T. Halpin-Healy and Y. C. Zhang, Phys. Rep. **254**, 215 (1995).
[3] L.-H. Tang, in *Annual Reviews of Computational Physics II*, edited by D. Stauffer (World Scientific, Singapore, 1995), p. 137.
[4] F. Family and T. Vicsek, J. Phys. A **18**, L75 (1985).
[5] A-L. Barabasi and H. E. Stanley, *Fractal Concepts in Surface Growth* (Cambridge University Press, Cambridge, England, 1995).
[6] M. J. Vold, J. Colloid Sci. **14**, 68 (1959).
[7] M. Kardar, G. Parisi, and Y. C. Zhang, Phys. Rev. Lett. **56**, 889 (1986).
[8] R. Jullien and P. Meakin, Europhys. Lett. **4**, 1385 (1987).
[9] S. F. Edwards and D. R. Wilkinson, Proc. R. Soc. London, Ser. A **381**, 17 (1982).
[10] Y. P. Pelligrini and R. Jullien, Phys. Rev. Lett. **64**, 1745 (1990).
[11] Y. P. Pelligrini and R. Jullien, Phys. Rev. A **43**, 920 (1991).
[12] F. Family, J. Phys. A **19**, L441 (1986).
[13] H. F. El-Nashar, W. Wang, and H. A. Cerdeira, J. Phys.: Condens. Matter **8**, 3271 (1996).
[14] H. F. El-Nashar, W. Wang, and H. A. Cerdeira, Surf. Sci. **391**, 1 (1997).
[15] H. F. El-Nashar, W. Wang, and H. A. Cerdeira, Phys. Rev. E **58**, 4461 (1998).
[16] D. Stauffer, Phys. Rep. **54**, 1 (1979); *Introduction to Percolation Theory* (Taylor & Francis, London, 1985).
[17] David Y. K. Ko and Flavio Seno, Phys. Rev. E **50**, R1741 (1994).