Dynamic scaling in a ballistic deposition model for a binary system

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A ballistic deposition model for the kinetics of surface growth for two species is introduced as a description of the evolution of a surface under vapor deposition. We used a tunable parameter P to control the deposition of the particles such that one type is deposited with probability P while the other is deposited with $1-P$. Simulations in $2+1$ dimensions using local surface diffusion lead to the formation of a rough surface whose dynamical evolution is not that of the Kardar-Parisi-Zhang universality class. Also, when surface diffusion becomes dominant, the model moves away from the Edwards-Wilkinson universality.

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The growth of surfaces by vapor deposition and its mechanisms have been extensively studied in the past [1,2] motivated by technological applications. Most previous studies have dealt with the growth of deposited components of only one kind. However, since growth of two or more species is common in modern technology, the study of such of problems has great interest which extends to its relevance in understanding nonequilibrium statistical mechanics, since the growth process may belong to a new universality class [3–5].

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 and 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 [1] is given by

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

The roughness exponent α and the growth exponent β 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 [1,2]. Many of these models belong to the Kardar-Parisi-Zhang (KPZ) universality class [6]. However, there have been many efforts to discover different universality classes.

Even though models of surface growth for binary systems have been presented in previous work [3–5,7], little is known about the kinetic roughening originating in these models and our understanding of this kind of growth is still in an early phase. Among the models used to represent the growth of composite systems, a well studied example is the ballistic deposition (BD) model. Here, particles rain down vertically onto a substrate and join the aggregate at the point of contact, giving rise to a rather interesting structure: The surface is a self-affine fractal although the bulk, which is filled with voids inside, is compact [1]. The BD model captures the essential features of processes such as vapor deposition. However, 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 out the surface [1]. Therefore, to simulate deposition as realistically as possible, both diffusion and overhangs/voids must be included [4,8]. Thus, in the growing system, there may exist different kinds of interactions for the two species in addition to the overhangs and diffusion, which in turn yield a different kinetics of growth associated with a change in the morphological structure of the aggregate. Pelligrini and Jullien [7] described surface growth according to a model with two kinds of particles, sticky and sliding. 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 [9], i.e., a model with surface reconstruction that belongs to the Edwards and Wilkinson (EW) universality class [10], while, when $c=1$, it is equivalent to the plain ballistic model that fits in the KPZ universality class. However, they do not present a kinetic study and how the surface evolves with time to a steady state. In a previous report [4] we have used a BD model for two kinds of particles (active and inactive) including diffusion on the surface where we allowed the following interactions: the active particle falling over a given column (or site) always sticks over an active particle, or it sticks over an inactive particle when there is an active particle among the nearest neighbors of the chosen column one layer higher than the inactive one. Diffusion to a local minimum around the neighborhood of the chosen site is introduced when an inactive particle deposits over an active one or deposits over an inactive particle with an active particle among the nearest neighbors one step higher. We found a morphological structural transition as the probability of be-

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ing an inactive particle increases. Although we introduced surface diffusion in the BD model, the values of the extracted exponents do not give an indication that the universality is changed from KPZ to EW type. Such a transition is attributed to the presence of three different processes during growth; overhanging, nonlocality, and surface diffusion. The competition between these three processes finally leads to a different kinetics.

In this paper, we focus our studies on kinetic roughening, scaling, and morphologies in a model for binary systems. Such a study may help to understand to which universality class the model belongs. We concentrate on the situations where surface diffusion is introduced for both types of species. We use a BD growth model which includes surface relaxation for both components. We introduce interactions between the two species since one kind is necessary for the deposition to occur, while the presence of the other kind allows diffusion to take place. This in turn may lead to an elimination of the nonlocal growth and formation of more voids under the surface [4]. Here, we present results of numerical simulations for the growth kinetcs and morphology in $2+1$ dimensions. We use the probability P as a continuously tunable parameter to control the system, where the deposition of two species occurs as $(1-P)$ for one type of component and P for the other type.

The model in this work is based on the BD model, which is composed of two kinds of particles A and C, with nearest neighbor interactions between particles. The deposition occurs on a substrate of size L^2 with probabilities $1-P$ and P for particles A and C, respectively. Surface diffusion is introduced for both types of particles since it plays an important role from the point of view of applications to real growth processes. We do not allow reconstruction processes in the bulk since the rate of this kind of process is much lower than the rate of processes on the surface. Also, we do not include evaporation processes in the model since deposition occurs more frequently than evaporation. The model we propose is appropriate to describe reactions that take place on the growing surface of materials. It represents the surface growth of a material with a low concentration of impurities. These impurities are represented by particles C, which have fewer active bonds than particles 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). Diffusion results when a particle deposits over one of a different type, that is, particle A deposits over particle C or particle C deposits over type A. In general, the presence of particle A is important for deposition to happen while type C is allowing diffusion to appear. A cross section of the aggregate is shown in Figs. 1(a) and 1(b). The white squares represent the aggregated particle 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

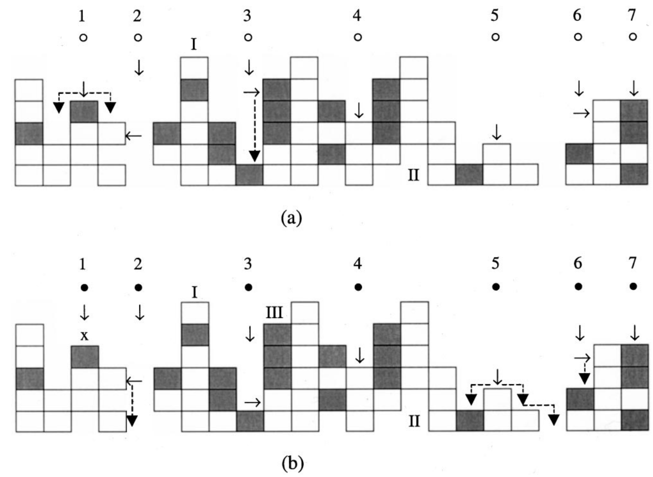

FIG. 1. A cross sectional piece of the aggregate. White squares stand for particles A and dark squares symbolize particles C. (a) The empty circles denote the deposited particles of type A. The deposition is indicated by the arrows. The diffusion process is denoted by fallen particles 1 and 3. (b) The full circles represent particles of type C. The deposition is indicated by arrows. The process of diffusion is represented by fallen particles 2, 5, and 6.

particle A that meets, either at the top of the chosen column (particles 4 and 5) or sideways (particles 2 and 6); on the other hand, if no particle A is found the incoming particle sticks to the top of the chosen column and then diffuses (particles 1 and 3) or remains on it if the neighbors are at equal or higher height (particle 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 is discarded if it finds a particle C and there are no particles A along the neighboring columns higher by one step (particle 1); on the other hand, if the chosen column is lower than its neighbors and the highest neighbor contains a particle A, the particle will diffuse if there is at least one neighboring column lower than the chosen one (particle 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 the chosen site if it finds a particle A either at the top (particle 4) or sideways (particles 3), otherwise the particle will be discarded (particle 1). In Fig. 1, particle 7 represents the border of the surface and we should interpret the last column depicted as a neighbor to the first one due to the boundary conditions. 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, or because of diffusion. Also a process of type II occurs due to lateral sedimentation at any one of the four neighbors 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.

We performed simulations for this model on a square lattice with $d=3$. The aggregation occurs in the Z direction with periodic boundary conditions in the X and Y directions. The statistical average is obtained over 500 independent simulations for each parameter.

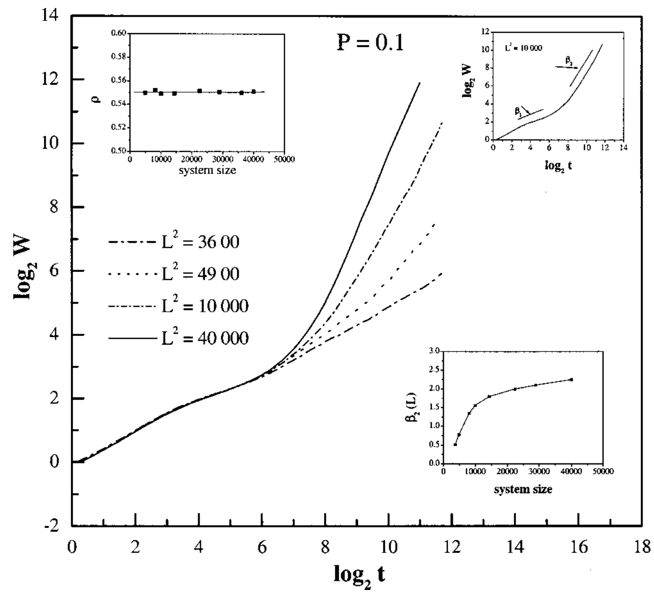

FIG. 2. Log-log plot of the surface width versus time for $P = 0.1$ and for different system sizes. The upper left inset shows the density versus system size. The upper right inset shows the existence of the two regime growth exponents when $L^2 = 10\,000$. The lower inset shows $\beta_2(L)$ versus different system sizes.

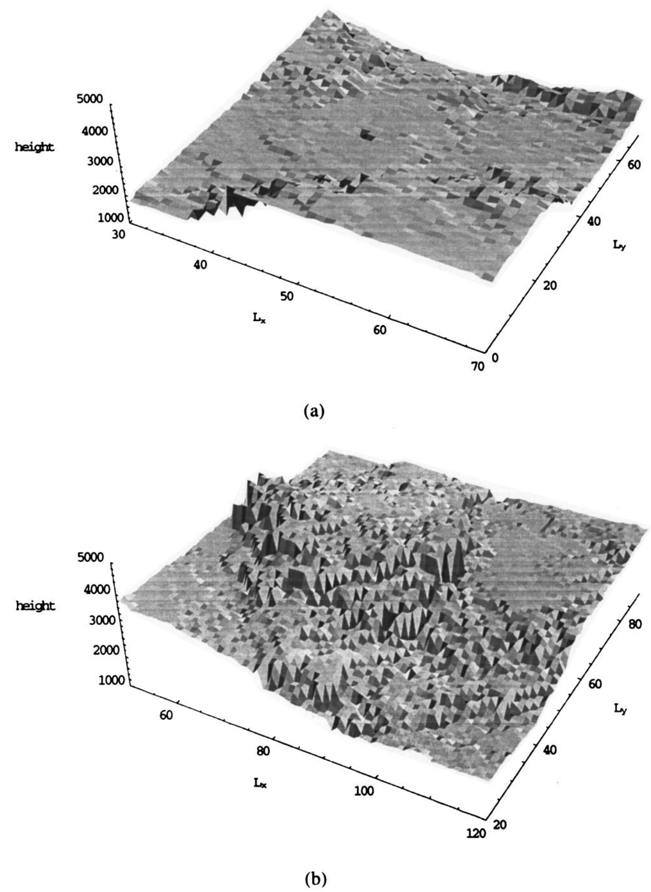

FIG. 3. Three dimensional plots of the surface with different system sizes for $\log_2 t = 10.5$; (a) $L^2 = 10\,000$ and (b) $L^2 = 40\,000$.

Figure 2 shows a log-log plot of the surface width W as a function of the time of growth t (number of deposited layers) for a probability $P = 0.1$ for different lattice sizes. We observe surprising results: the surface width (roughness) W increases as a function of t during three different stages. In the first stage, where $1 < \log_2 t < 3$, roughness enlarges as $W(t) \sim t^{0.53}$ and this stage may be considered as a transient [2]. During the second stage the surface width grows as $W(t) \sim t^{\beta_1}$ where $\beta_1 = 0.37$ for all system sizes. Later, the surface roughness extends as $W(t) \sim t^{\beta_2(L)}$, where $0.52 \leqslant \beta_2(L) \leqslant 2.25$ for $3600 \leqslant L^2 \leqslant 40\,000$. The upper right inset of Fig. 2 shows clearly the two growth exponents for a system size $L^2 = 10\,000$. It is clear from the figure that as the time increases the surface width does not reach saturation. Simulations (with less statistics due to computational limits) for larger times than those presented in Fig. 2 show that W does not reach saturation. In an attempt to interpret the above results, we have investigated the morphology. Figures 3(a) and 3(b) show a surface view taken at $\log_2 t = 10.5$ for two values of system size, $L^2 = 10\,000$ and 40 000, respectively. The figure reveals that the surface has a rough structure which becomes rougher as the system size increases. The values of both exponents suggest that there are two regimes of growth: one at intermediate times and one at long times. Also, for the larger system size deep and large grooves are formed over the surface, resulting in large fluctuations of height. Thus, surface width grows having an exponent $\beta_2(L) \gg \beta_1$. The reason for the sudden steep slopes over the surface, which increase with system size, can be explained as follows. During growth, the deposition of type A is more frequent than that of type C. Diffusion is allowed for type C more than for type A since it is more probable that A will find another particle A to stick to it than a C type. In addition, if A sticks to C it diffuses to a local minimum in the neighborhood of the chosen column. Therefore, over the areas covered by C, diffusion is more frequent, while over the areas of A type, adhering is dominant. Also overhangs become more common along the columns of the areas of type A, since the areas of type A grow faster than those of type C. These effects lead to a surface with steep slopes where the growth exponent is high. Figures 4(a) and 4(b) show a section of area equal to 10 000 where the distribution of particles over the surface for system sizes 10 000 and 40 000 is shown at $\log_2 t = 10.5$. We notice from this figure that the areas of type C increase as size increases. So wide areas over the surface grow at a slower speed. Finally, deep grooves are formed which become wider as system size increases. Also, the overhangs along the columns that contain particles of type A increase the growth rate along these columns. Figure 2 shows that the density ρ for the long time limit (the top left inset), where $\rho = N/\langle h \rangle L^2$, remains constant when the system size increases for the same value of P, strengthening the argument above that overhanging is common and has the same contribution for all system sizes. Figure 5 shows a log-log plot of the surface roughness versus time for values of the probability $0.1 \leqslant P \leqslant 0.3$ when the system size equals 10 000. This figure reveals that the saturation of the surface width in the long time limit can be defined for $P \geqslant 0.18$ (see the left inset of Fig. 5). We argue that this behavior is due to the balance, in the long time limit, between diffusion and overhangs. That is, diffusion competes with overhangs/voids and drives the surface width to saturate earlier (during the first regime). Within the second regime overhangs dominate

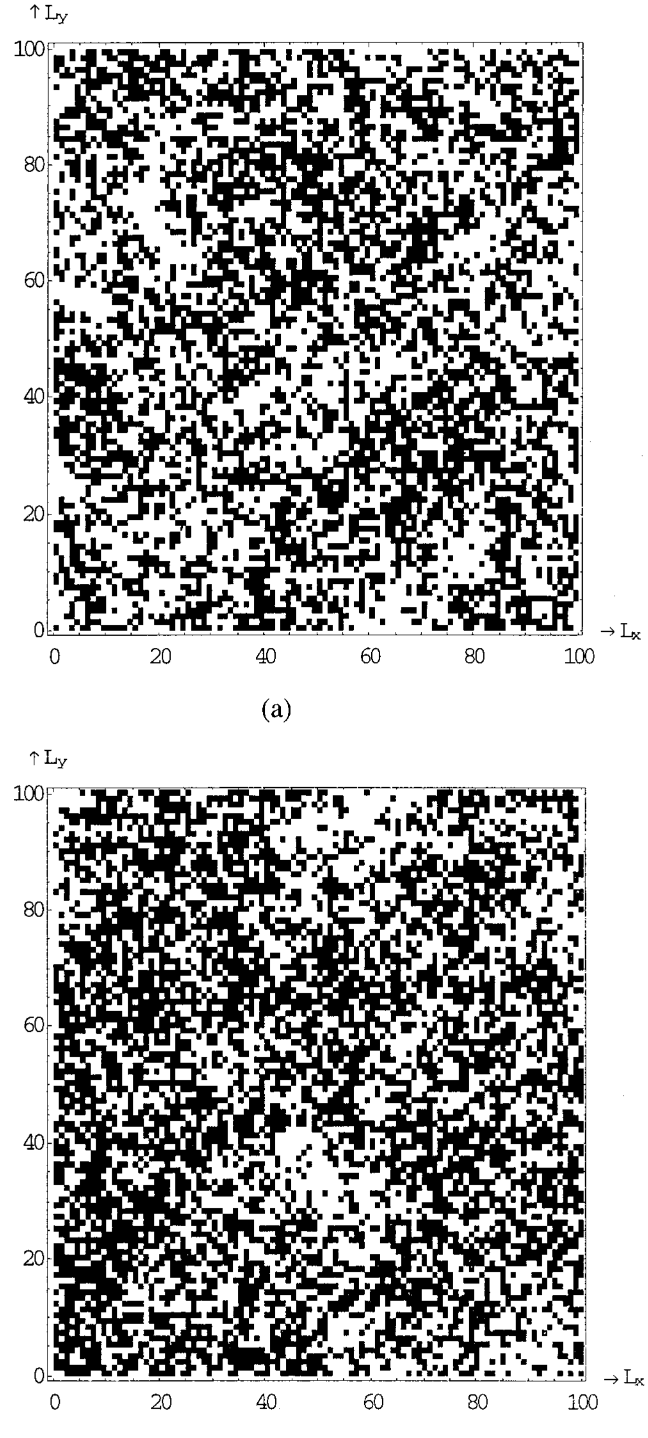

FIG. 4. View of the distribution of particles over a section of the surface of size 10 000, where type A is white and type C is black, for $\log_2 t = 10.5$ and for two system sizes, (a) $L^2 = 10\,000$ and (b) $L^2 = 40\,000$.

and increase the growth rate. However, the two regimes of growth are present for $P < 0.3$ as indicated from the right inset of Fig. 5, while the left inset shows the presence of the two regimes of growth at $P = 0.2$. For $P \geqslant 0.3$ there exists only one regime of growth with a single value of the growth exponent β. Figure 6 shows a log-log plot of W versus t when $P = 0.4$ and for different system sizes. It is apparent

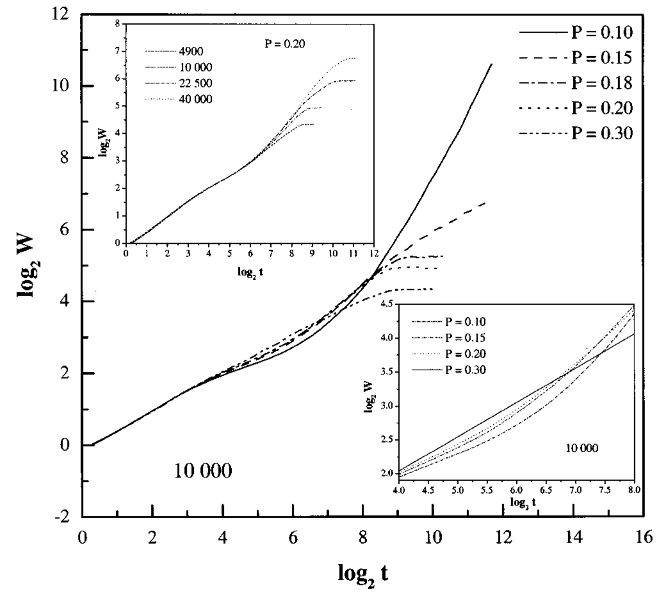

FIG. 5. Log-log plot of the surface width versus time for $0.1 \leqslant P \leqslant 0.3$ for system size $L^2 = 10\,000$. The left inset shows the surface width versus time for $P = 0.2$ for different system sizes. The right inset shows the presence of the two regimes of growth for $P < 0.3$ when $L^2 = 10\,000$.

from this figure that only one value of β is extracted. The inset of Fig. 6 shows how the exponent α is determined. The values of $\alpha = 0.51$ and $\beta = 0.49$ point to a columnar growth morphology at this value of P resulting from the presence of void formation and diffusion processes. Voids enhance the growth rate in the areas of type A while surface diffusion slows down the growth rate of areas that include type C. Therefore, a surface with a slightly larger fluctuation in height appears, as indicated from the values of the exponents. Figure 7 shows a log-log plot for the surface roughness versus time for different values of the probability $0.3 \leqslant P \leqslant 0.999$. This figure shows that a decrease in the surface

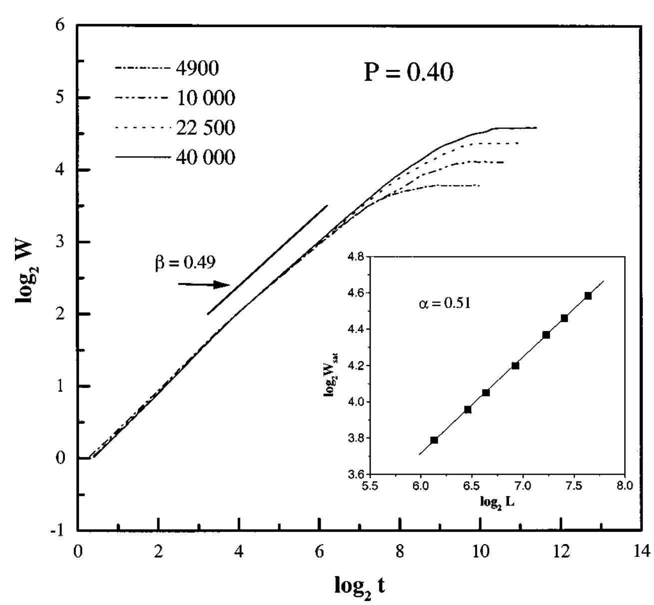

FIG. 6. Log-log plot of the surface width versus time for $P = 0.4$. The inset shows a log-log plot of W_{sat} versus L.

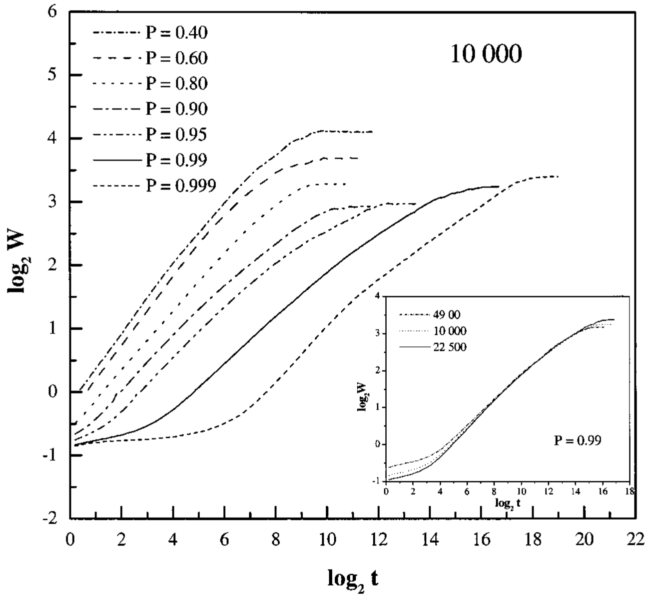

FIG. 7. Log-log plot of the surface width versus time for $0.4 \leqslant P \leqslant 0.999$ for $L^2 = 10\,000$. The inset shows W versus t for $P = 0.99$ and for different system sizes.

width happens as P increases. It is also seen that W has the same trend for $0.4 \leqslant P \leqslant 0.6$. For $P \geqslant 0.8$ it becomes apparent that the surface width saturates at longer times. For $P > 0.95$ the kinetics change and the surface width saturates at a very long time. The inset of Fig. 7 indicates that the surface width grows with time, having an exponent β, and we are able to define an exponent α when $P = 0.99$. Also as shown in Fig. 7, even for $P = 0.999$, W increases with time until it saturates, giving an indication of a power law growth during the intermediate time. At this limit of P we could not extract values for the exponents α and β due to a computational limit for large system sizes. Here, diffusion becomes greatly dominant since particles of type C deposit much more often than those of type A. However, the presence of type A allows the growth to continue, where some voids are formed under the surface that could not be eliminated by surface diffusion. Therefore, the surface grows at a low rate and takes a long time to reach saturation. According to the rules of the model, when $P = 1$, all deposited particles are of C type and no deposition occurs, since we do not allow deposition of particles C over C. Figures 8(a) and (b) show the values of the exponents α and β, which are plotted versus the probability P. The values of exponents from both plots of Fig. 8 show that as P increases the exponents decrease. This means that, upon increasing the diffusion processes on the surface, the fluctuation in height decreases and the aggregate formed has fewer voids inside. Both plots also indicate that for $0.6 \leqslant P \leqslant 0.8$ the values of both exponents are approximately constant. This points to a surface with approximately the same morphology within this interval and a balance between overhangs/voids and diffusion occurs through the growth stages. Also, both plots show that at $P = 0.99$, where surface diffusion becomes significant, the values of the exponents are $\alpha = 0.21$ and $\beta = 0.26$. These values are small and they indicate that surface diffusion diminishes the formation of voids under the surface. It is well known in the model with surface relaxation that the exponents $\alpha = \beta = 0$ and the

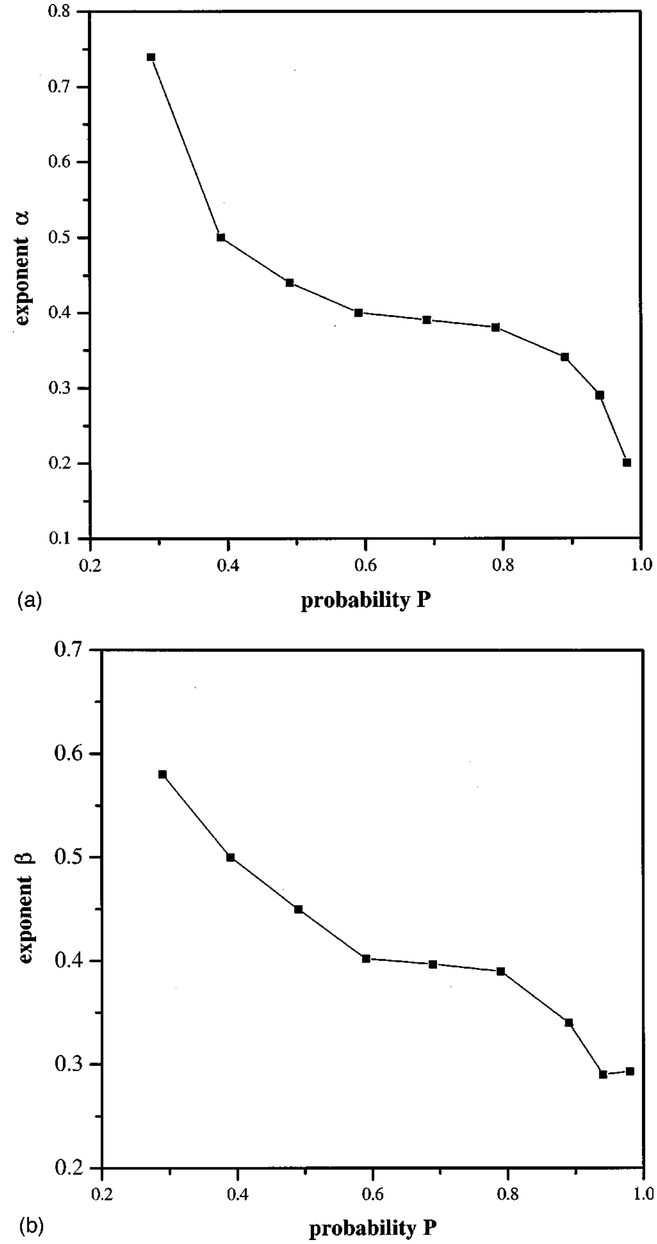

FIG. 8. (a) The exponent α versus the probability P. (b) The exponent β versus the probability P. Note that the lines in both figures are drawn for convenience.

model belongs to the EW universality class [1,2,10]. However, both exponents show that, in $2+1$ dimensions in our case, when $P = 0.99$ the width scales nonlogarithmically with time and the saturation width does not depend on the logarithm of the system size. Although we used the ballistic deposition model for two species which tend to the usual BD model when $P = 0$ and follow KPZ universality, we do not observe the features of this universality when we switch on the parameter P, even for smaller values of P. Also, when diffusion dominates, the values of α and β do not approach zero and the model does not belong to the EW universality class.

To complete the study of these kinetics we have measured the average velocity of the interface as the value of P increases. Figure 9 shows a plot of the average velocity versus $\log_2 t$. It is clearly seen that, for $P = 0.1$, the velocity de-

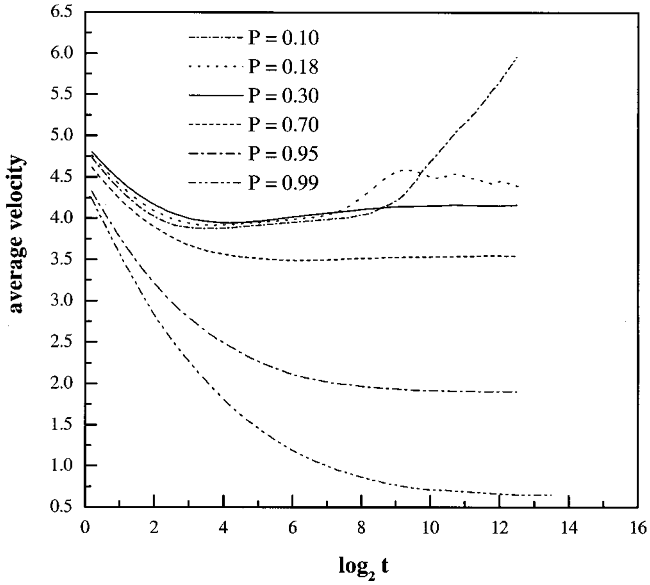

FIG. 9. The average velocity as a function of time for different values of P when $L^2 = 10\,000$.

creases, and it seems that the interface is driven to saturate due to the presence of diffusion, at the intermediate time, which tries to overcome the overhangs/voids. However, due to the presence of more particles A than C, the voids under the surface increase the rate of growth and the effect of diffusion in the long time limit becomes smaller. This enhances the growth and finally the velocity increases. When P approaches 0.2 the diffusion process becomes somewhat more important, and in the long time limit, although the void formation tries to drive the interface with higher velocity, the diffusion balances it, slowing the growth rate until the surface width saturates. For $0.3 \leqslant P \leqslant 0.99$, the average velocity has the same features but with lower values at saturation; it does not approach zero however. Figure 10 shows the density of the aggregate when it is plotted versus P for system size equal to 10 000. The figure shows that the density in-

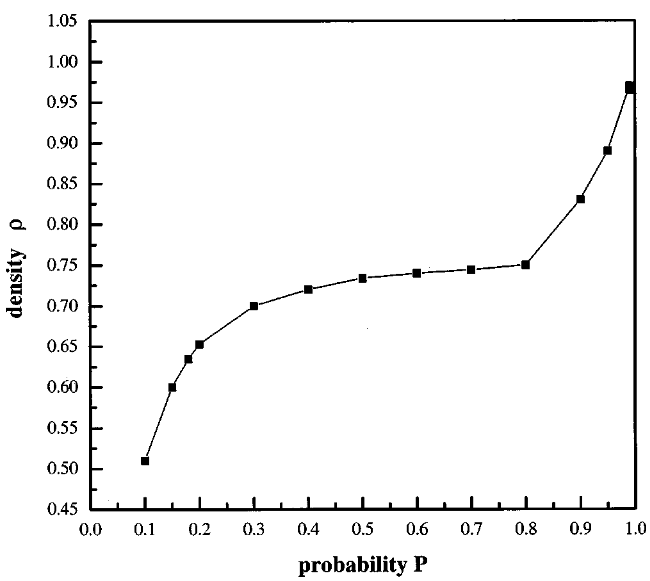

FIG. 10. The density ρ versus the probability P for $L^2 = 10\,000$. Connecting line is drawn for convenience.

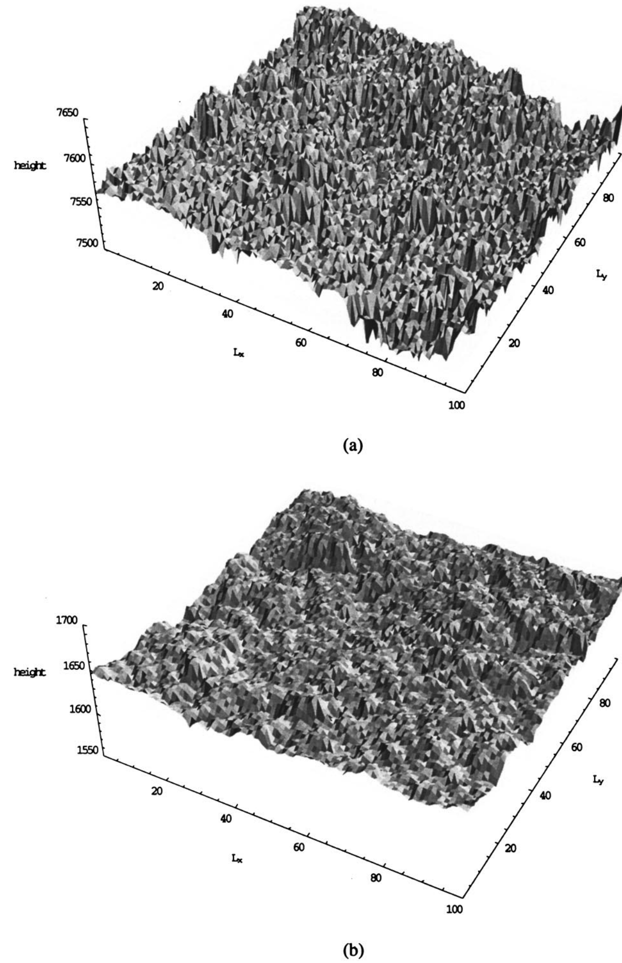

FIG. 11. Three dimensional plots for the surface at saturation for two different values of P and for $L^2 = 10\,000$; (a) $P = 0.3$ and (b) $P = 0.99$.

creases rapidly as the value of P increases for $0.1 \leqslant P \leqslant 0.2$, while it increases little for $0.3 \leqslant P \leqslant 0.8$. Then the density increases more for $P > 0.8$. It is revealed from Fig. 10 that the voids are formed more under the surface for small values of P. This result is due to formation of more overhangs during growth while diffusion takes place only over small areas on the surface. As P increases the diffusion process tries to equate the overhangs/voids, leading to the previous kinetics of Figs. 5 and 7. For $P \geqslant 0.99$, the value of the density $\rho \approx 0.96$ shows that the formation of overhangs/voids is still occurring. Such processes cause the lateral and perpendicular correlations to grow nonlogarithmically with system size and time, respectively. Figures 11(a) and (b) show surface plots for $P = 0.3$ and $P = 0.99$, respectively. It is observed that for $P = 0.3$ the morphology is dominated by columnar growth and a surface of notable fluctuations in height is formed (as indicated by the large values of α and β). For $P = 0.99$ the morphology reveals that the surface is smooth due to relaxation, which makes the surface width grow with small values of α and β. So the importance of allowing diffusion for the active particle to smooth the surface is shown clearly in the pictures of Fig. 11, in addition to its role in eliminating the nonlocality described in Ref. [4].

All of the above results prompt us to argue that, upon introducing diffusion to the BD model for a binary system, the behavior of kinetic roughening as well as the morphological structure are changed. Although we used a BD model with surface relaxation, which reduces to the usual BD model that follows KPZ universality, we observed a change in universality after switching on the parameter P and allowing diffusion for both particles. As P increases and the diffusion processes over the surface become dominant, the values of the exponents decrease, giving an indication of a smoothing of the surface due to relaxation. However, as P approaches unity the values of the exponents do not approach zero, as in the case of a BD model with surface diffusion [7], and the model does not belong to the EW universality class.

Our results lead to a conclusion that in $2+1$ dimensions there may be a different universal behavior for models of binary systems. However, in order to clarify this argument and to determine which universality class our model belongs to, a further detailed study of correlations is required.

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