Growth morphology for a ballistic deposition model for multiple species

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The kinetics and morphology of surface growth are studied for a ballistic deposition model with two kinds of particles (A and C) in $1+1$ and $2+1$ dimensions. A morphological structural transition is found as the probability of being a particle C increases. This transition is well defined by the different behavior of the surface width when it is plotted versus time and probability. The calculated exponents α and β for different values of probability show the same behavior. We attribute this transition to the formation of wide vacancies during the growth while the interface advances. [S1063-651X(98)02008-X]

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I. INTRODUCTION

The growth of surfaces and interfaces remains a challenging problem in physics. It attracts much interest due to its technological importance as well as its relevance in understanding nonequilibrium statistical mechanics at the fundamental level [1–3]. The study of the kinetics of crystal growth helps us understand this phenomenon since it describes how the surface evolves with time, while the study of the morphology provides a clear interpretation of the growth. Most of the studies contain rough surfaces and stochastically growing interfaces in the context of the ballistic deposition (BD) as well as other models and continuum growth equations [4].

A different feature of this phenomenon is the existence of dynamic scaling [5], i.e., if we start at $t=0$ from a flat substrate of length L, we have

$$W(L,t)=L^{\alpha}f(t/L^{z}), \tag{1}$$

where $W(L,t)$ is the surface width

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

Here $h(r,t)$ is the height of the surface at position r and time t, $\overline{h(t)}$ is the average height at time t, and $d'=d-1$ is the substrate dimension. The dynamical scaling behavior is characterized by the roughness exponent α and the dynamical exponent β with $z=\alpha/\beta$. The scaling function $f(x)$ behaves as $f(x)=x^{\beta}$ for $x\ll 1$ and $f(x)=$const for $x\gg 1$. The scaling behavior has been studied in various systems and models and has been argued to be universal [1–4]. One of the successful theoretical approaches describing the BD model is that of Kardar, Parisi, and Zhang [6], which is based on Edwards and Wilkinson's theory [7]. The Kardar-Parisi-Zhang equation is a nonlinear Langevin equation

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

for the local growth of the profile $h(r,t)$ of a moving interface about a d'-dimensional flat substrate.

The BD model represents an example of well studied growth models. Here particles rain down vertically onto a d'-dimensional substrate and aggregate upon first contact [8]. Such a model gives rise to a rather interesting structure: The surface is a self-affine fractal, although the bulk is compact [3]. Most previous studies have dealt with the surface growth of one kind of particle [1–4]. Generally, in the growth of real materials one should take into consideration that different kinds of particles are deposited. Thus, in the growing system, there may exist different interactions for different particles, which in turn yield a different kinetics of growth associated with a change in the morphological structure of the aggregate. Pelligrini and Jullien (PJ) [9,10] described a surface growth according to a model with two kind of particles, sticky and sliding, where both are active. This model interpolates between a diffusive model that 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 [11], i.e., a model with surface reconstruction, while when $c=1$ it is equivalent to the plain ballistic model.

In our work we describe the kinetic growth in $1+1$ and $2+1$ dimensions as well as the morphological structure in order to interpret the results that have been obtained from the kinetics for two kinds of particles that are active and inactive. We hold the growth rules of the ballistic model for different condition and in all cases [12–14]. So we do not introduce any kind of surface diffusion for the inactive particles or any reconstructuring processes on the surface. In $2+1$ dimensions, which simulates the real surface growth, we extend the interaction between particles from nearest-

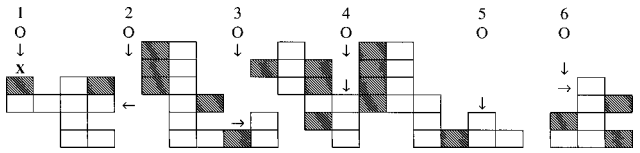

FIG. 1. Ballisticlike deposition model of two kinds of particles. The white rectangles represent particles A and the dark rectangles denote particles C. The circles refer to incoming particles (A or C). The arrows indicate the path of the particles where it sticks.

neighbor (NN) to next-nearest-neighbor (NNN) interactions in order to see this effect on kinetics. We use the probability P as a continuously tunable parameter to control the system. We find that there is a transition for both dimensions: Above a critical probability P_c the growth kinetics has different features from below P_c and it is attributed to the change in the morphological structure of the system.

The arrangement of the paper is as follows. In Sec. II the ballistic deposition model for two species is described. The kinetics of growth and the morphological structure are presented in Secs. III and IV, respectively. Finally, a conclusion is given in Sec. V.

II. A BALLISTIC DEPOSITION MODEL FOR TWO SPECIES

Two different kinds of interacting particles, particle A (the active particle) and particle C (the inactive one) with probabilities $1-P$ and P, respectively, are deposited on a substrate of size $L^{d'}$. The particles are allowed to fall randomly straight down, one at a time, onto a growing interface. At first, a column is selected at random and then particle A (or particle C) is deposited on the surface of the aggregate with a probability $1-P$ (or P). The clusters of the aggregate, separated by empty spaces are shown in Fig. 1. The white rectangles represent the aggregated particles of type A and dark rectangles represent those of type C. The incoming particles are denoted by circles, which mean both types of particles A and C. The path of the fallen particle is shown by the arrows. The deposition occurs according to the following processes. (a) If the dropping particle meets particle A on the top of the selected column, higher than its neighbors, the incoming particle sticks to it (fallen particle 5 in Fig. 1). (b) If the selected column is lower than any one of its neighbors, the incoming particle sticks on the side of any one of the neighboring columns when it finds particle A regardless of the type of particle on the top of this chosen column (fallen particles 2, 3, and 6 in Fig. 1). (c) If the chosen column is lower than its neighbors that have only particles C along them, the fallen particle continues downward and it sticks on the top of the chosen site if and only if it contains a particle A; otherwise it is discarded (fallen particle 4 in Fig. 1). (d) When the newly arriving particle (A or C) meets particle C on the top of the chosen site the particle does not stick and this process is excluded, except when the neighboring column contains particle A one step above the top of the chosen column (fallen particle 3 in Fig. 1).

It might be considered at first sight that our model is similar to the one proposed by PJ [9,10]; however, they are completely different. In their work the authors describe a surface growth according to a model with two kind of particles, sticky and sliding, where both are active. This model interpolates between a diffusive model that 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 [11], while when $c=1$ it is equivalent to the plain ballistic model. We do not expect that introducing the parameter P in our model will reproduce the same effect as in that of PJ since we do not include surface diffusion for the inactive particles.

We have chosen the model since it describes chemical reactions that 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. Particle A is chosen with a probability $1-P$ and 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 a low concentration of impurities. These impurities are represented by particle C, which has less active bonds than particle A. Further, 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 aggregation might be considered as a kind of percolation of the particles [15]. 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. GROWTH KINETICS

To perform simulations for this model, a lattice of size $L^{d'}$ is considered. The aggregation occurs in the Z direction. At the beginning all sites are occupied by particles A for $Z \leq 0$. Periodic boundary conditions are used in the X direction in $1+1$ dimensions and in both the X and Y directions in $2+1$ dimensions. The statistical average is obtained over 500 independent simulations for each parameter. We find that in $1+1$ dimensions for the system size $L<100$, the surface width is size dependent [12], while in $2+1$ dimensions only the system with NN interactions has this feature for $L<70$ [13,14]. Thus, in this work we always use a system large enough so that the results will not depend on size.

Figure 2 shows a log-log plot of the surface width W as a function of time t (the number of deposited particles) for different values of the deposition probability P and fixed system size. It is seen from this figure that the width of the surface first increases fast and finally saturates to a fixed value after experiencing a slowing down. For $P=0$, in all cases, the curve represents the usual BD model for only one kind of particle [12–14]. For small values of $P \neq 0$, the surface width becomes smaller as the probability increases and the saturation state is reached early. However, for $P>0.25$ in $1+1$ dimensions and $P>0.5$ in $2+1$ dimensions, the surface width increases as the time increases and the system saturates faster. In $1+1$ dimensions it is not possible to ex-

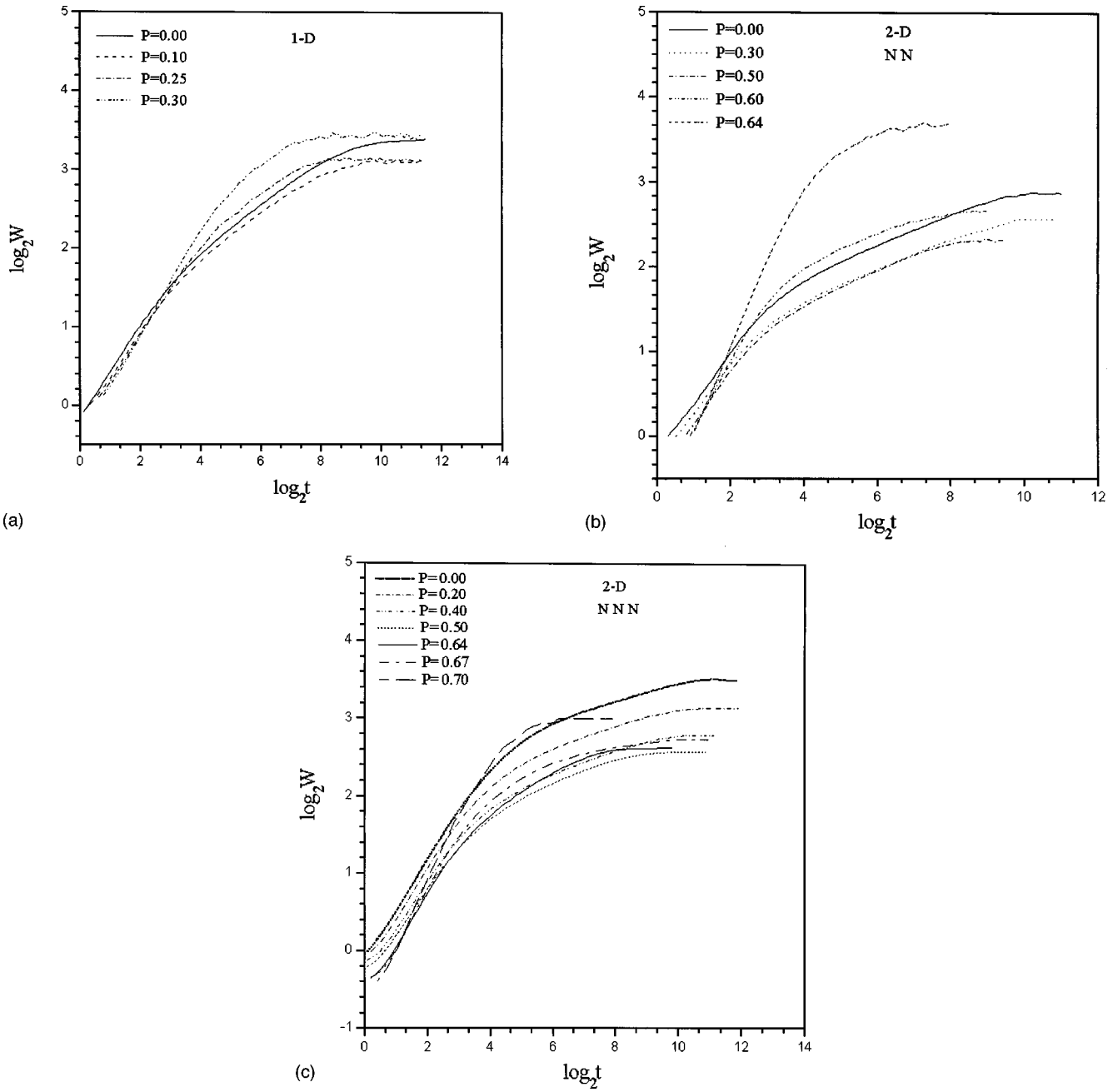

FIG. 2. $\log_2 W(t)$ versus $\log_2 t$ in (a) $1+1$ dimensions, (b) $2+1$ dimensions with NN interactions, and (c) $2+1$ dimensions with NNN interactions.

amine the system with high values of P due to the disappearance of bonds between particles after $P=0.32$, while in $2+1$ dimensions we are able to reach the values $P=0.64$ and 0.7 for systems with NN and NNN interactions, respectively. Figure 3 shows a plot of the logarithm of the saturation width $W(t=\infty)$ versus the probability P. It is shown that in each case the value of $W(t=\infty)$ first decreases as P increases and then it increases. The minimal point is found to be around $P=0.25$ in $1+1$ dimensions and $P=0.5$ in $2+1$ dimensions. Figures 4(a) and 4(b) show plots of probability versus the exponents α and β, respectively. The values of both exponents for $P=0$ give the same values in all cases for the usual ballistic deposition model [1,2,4,14]. It is shown in the figure that the exponents α and β do not change until $P=0.25$ and 0.5 for $1+1$ and $2+1$ dimensions, respectively. After these values of probability the exponent α increases for $1+1$ and $2+1$ dimensions with NNN interactions, while it decreases for the case with NN interactions. The exponent β increases for both cases after P exceeds 0.25 and 0.5 for $1+1$ and $2+1$ dimensions, respectively. It should be noted that both exponents becomes P dependent as P increases over the above-mentioned values.

Therefore, the different behaviors of the surface width and the exponents for different values of P led us to define a critical probability $P_c=0.25$ and 0.5 for $1+1$ and $2+1$ dimensions, respectively. The presence of this critical value indicates that a change in the morphological structure may happen when the value of P exceeds P_c. The rapid increase in the surface width after P_c may indicate that more voids are formed when the interface moves, which increases the

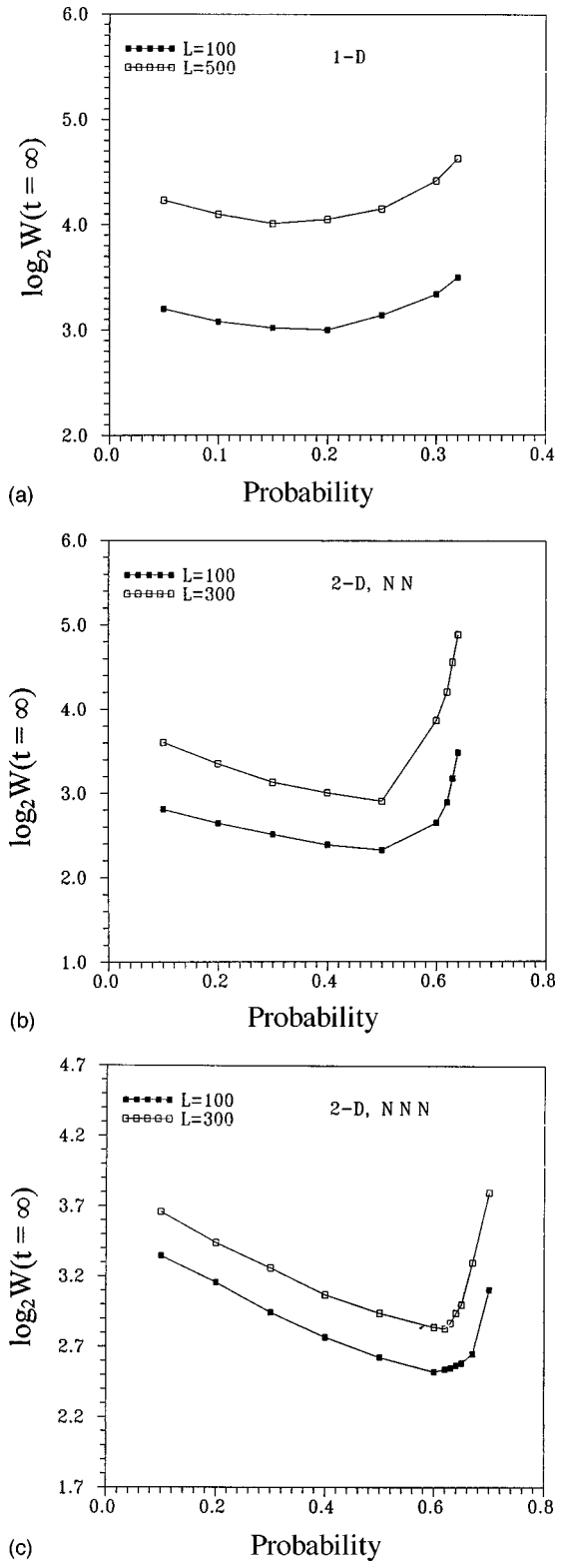

FIG. 3. $\log_2 W(t=\infty)$ versus the probability for different system sizes (the solid line joining the calculated points is drawn for convenience) in (a) $1+1$ dimensions, (b) $2+1$ dimensions with NN interactions, and (c) $2+1$ dimensions with NNN interactions.

nonlinear term $(\nabla h)^2$, since in the ballistic model the interface velocity depends on this term [4]. Furthermore, the values of the exponent α indicate that the surface becomes smoother for the model with NN interaction when P increases and rougher for the other two cases. In addition, the

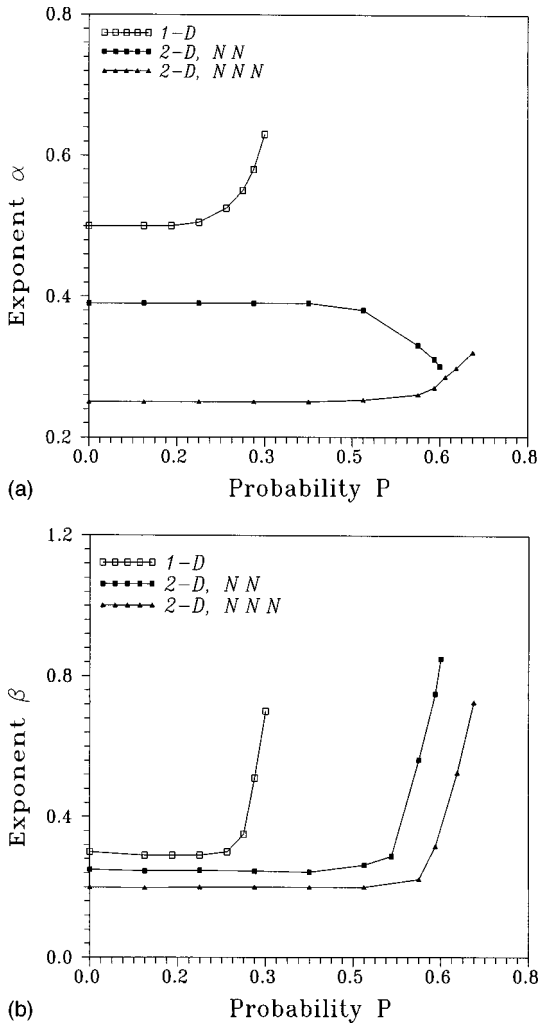

FIG. 4. Plot of the probability P versus (a) exponent α and (b) exponent β.

increase of the values of the exponent β after P_c in all cases implies high fluctuations in height [12–14], indicating a change in morphology. To make this argument more clear we need to study the density of the bulk, which will be done in the next section.

IV. MORPHOLOGICAL STRUCTURE

We conjectured in the preceding section that the kinetics of growth gives us an indication that as the probability of deposition of particles C increases, there exist two different morphological regimes separated by P_c. In order to interpret such features, the density ρ, where $\rho = N/\langle h \rangle L^{d'}$ and N is the number of columns, of the whole aggregate is calculated for each value of P in all cases. Figure 5 shows the densities of particles A and C as well as the total number of particles as a function of the probability P. We notice that the density of particles C increases and then decreases, while for particle A it decreases always, although faster after a certain P. This makes the whole density behave as the latter (particles A), indicating the formation of voids. After P_c, the number of voids formed increases due to the presence of more particles C, which introduce inert sites. Therefore, the presence of particles C enhances overhanging rather than downward dif-

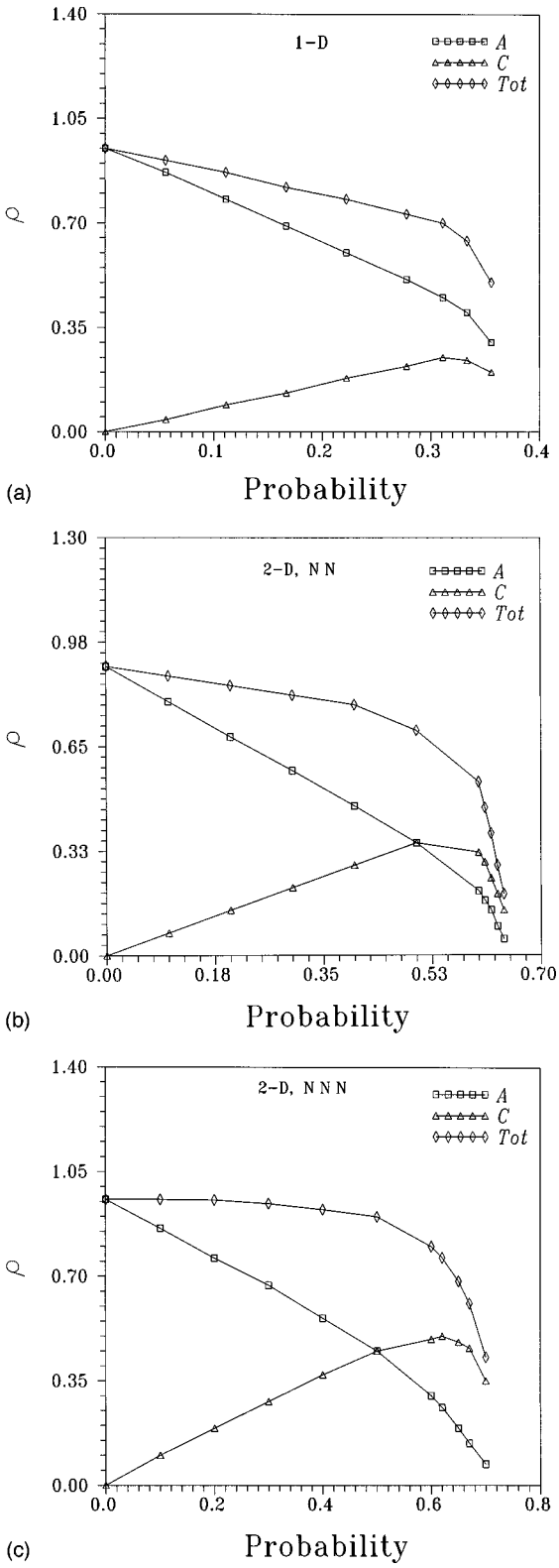

FIG. 5. Density of particles ρ against the probability P in (a) $1+1$ dimensions, (b) $2+1$ dimensions with NN interactions, and (c) $2+1$ dimensions with NNN interactions.

fusion as might be expected from the introduction of the model. Figures 6–8 show a cross-sectional view of the final part of the aggregates for $1+1$ and $2+1$ dimensions with NN and NNN interactions, respectively, for different probabilities. It is seen in these figures that the density of the bulk

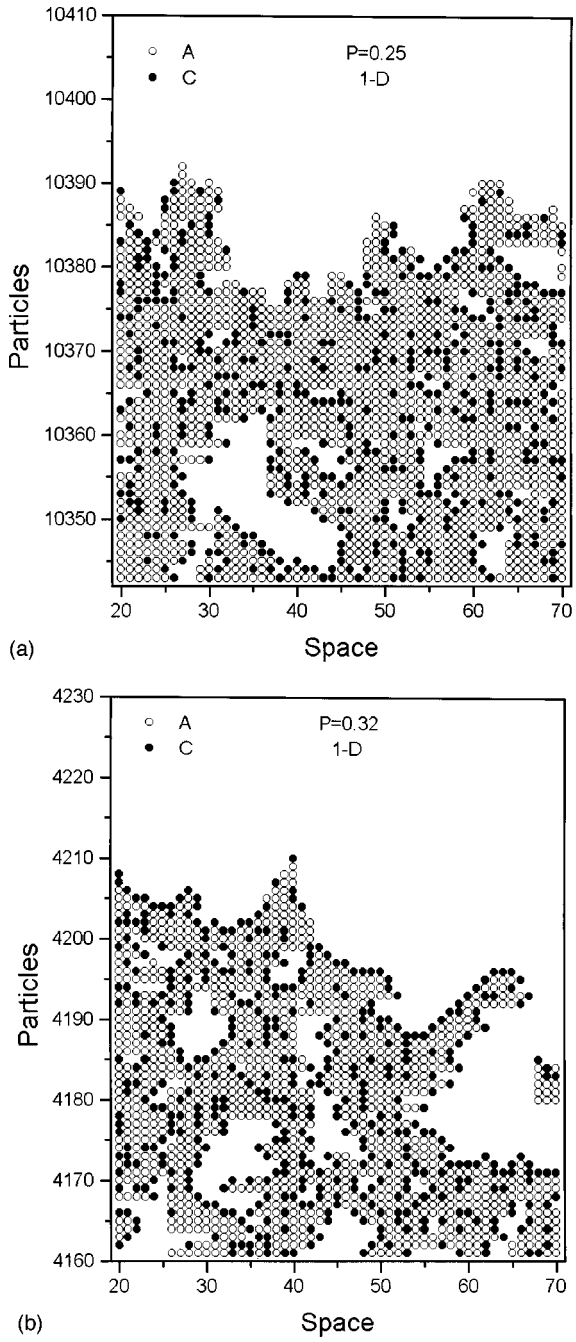

FIG. 6. Cross-sectional view of the final stage of the aggregates in $1+1$ dimensions for two different values of probabilities.

decreases when the value of P increases due to the formation of voids while the interface advances. Also, it is indicated in these figures that the connectivity of the particles is less above P_c.

Microscopically, the formation of such a different morphological structure in all cases can be understood as follows. For $P<P_c$ the deposition of particles of type A occurs more frequently than that of particles of type C. Since the bond strength between particles A is large, they are connected together forming big clusters separated by very small islands of particles C. This may lead to a rapid growth of the columns that contain particles A on their tops or along their neighbors that have more particles of type A through the sideways sticking and a slow growth of columns that contain

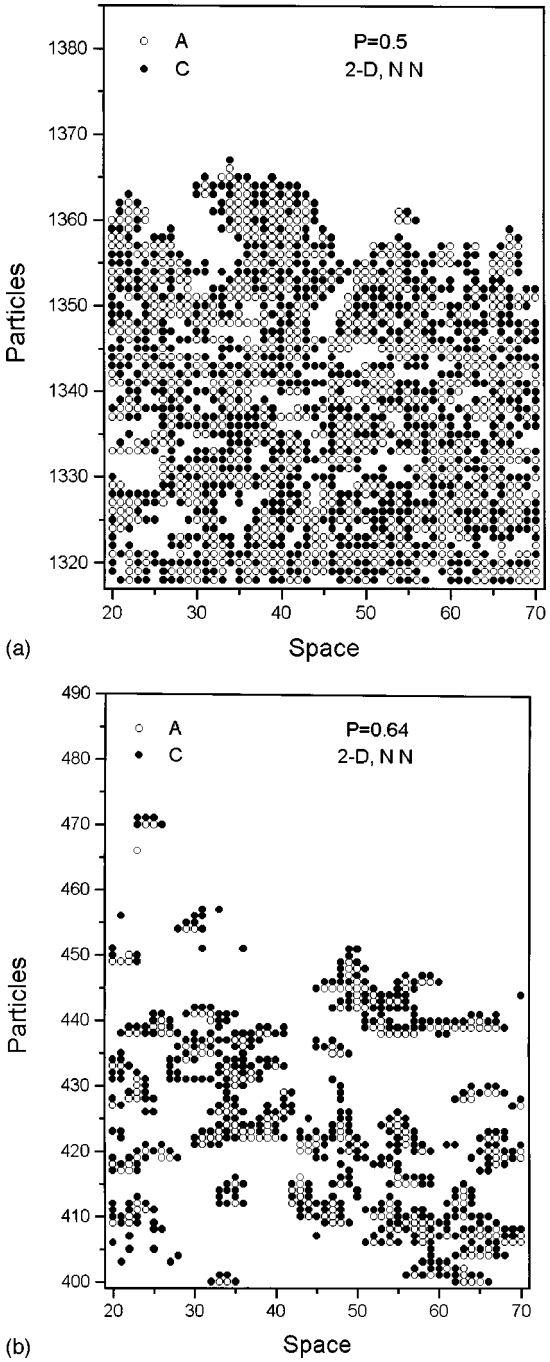

FIG. 7. Cross-sectional view of the final stage of the aggregates in $2+1$ dimensions with NN interactions for two different values of probabilities.

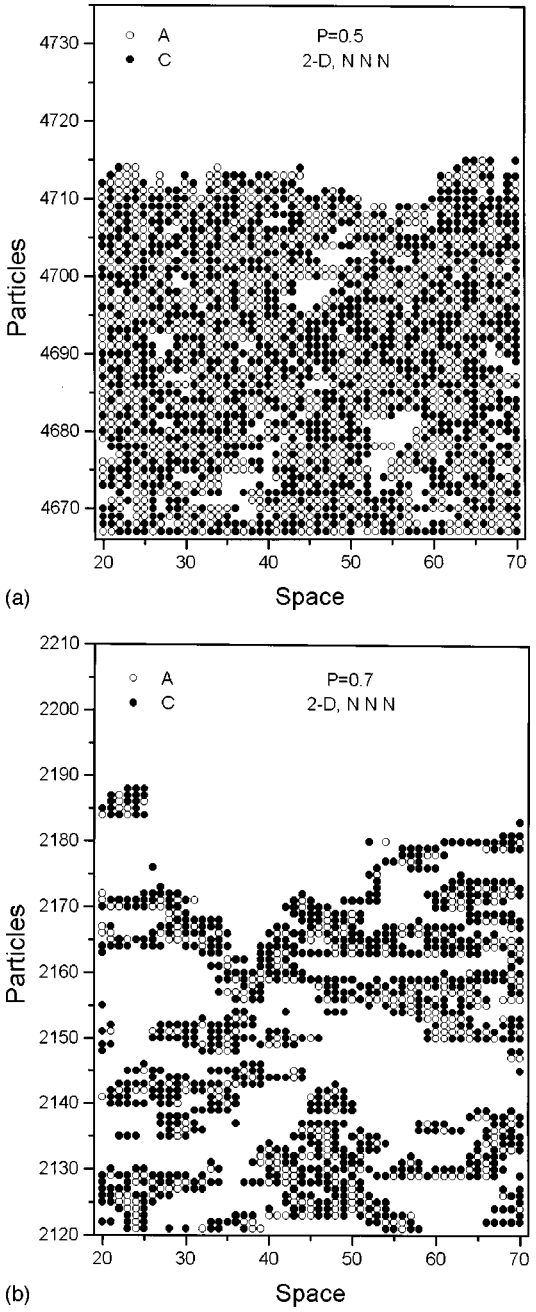

FIG. 8. Cross-sectional view of the final stage of the aggregates in $2+1$ dimensions with NNN interactions for two different values of probabilities.

particles C on their tops or along their neighbors. For $P > P_c$ there will be more particles C than A on the tops of the columns and on the neighbors. The incoming particle cannot move downward to encounter a particle A unless the neighbors 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 on the first. This may cause more overhanging processes, which enhances the lateral spreading of the surface [16]. This mechanism leads to an increase in the lateral correlation length, reaching the value of L faster; hence 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 perpendicularly to the local gradient, increasing the nonlinearity in the growing surface. However, in the case of NNN interactions, where the increase in the surface width after P_c is less than that of the NN case, there may exist a smaller increase in the surface gradient due to the extension of bond lengths. Then the formation of voids throughout the bulk is less in the NNN case than in the NN case [compare Figs. 7(b) and 8(b), noting that the first is for $P=0.64$ and the second for $P=0.7$]. In fact, when the interaction is extended to the NNN

sites, the chance for lateral sticking is increased since the probability of occupation of neighboring sites by particles A increases (note that the number of neighbors is 8). This in turn causes smaller formation of voids for small values of P and leads to an approximate constant density [see Fig. 5(c)]. This effect on the surface width and the interface velocity can be seen in Figs. 2 and 3 and while the kinetics of both cases of NN and NNN interactions have the same trend, the surface width goes to higher values in the case of NN than that of the case of NNN interactions.

V. CONCLUSION

In our simulations we have studied the kinetics and morphology of surface growth for different probabilities. We found that 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, these wide vacancies are responsible for the different growth kinetics above and below P_c.

In conclusion, we have proposed a ballistic surface growth model for deposition of two kinds of particles in 1 $+1$ and $2+1$ dimensions with NN and NNN interactions. A phase transition of the morphological structures has been found as the probability P increases. The physical origin of the transition lies in the tendency of particles C to aggregate together to form inert clusters and the different interaction processes between different particles. Also the presence of particles C increases the formation of voids, inducing a fast growth rate to earlier saturation of the surface width. Furthermore, the tendency of particles C (inert particles) to form clusters on the surface leads to a nonlocality in the growth where the flux of the particles is captured by some sites. This enhances the formation of wide and deep grooves on the surface due to the growth of some sites more than others. This effect is indicated by the higher values of the exponent β in all cases after P_c.

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