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A discrete surface growth model for two components

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Abstract

We present a ballistic deposition model for the surface growth of a binary species A and C. Numerical simulations of the growth kinetics show a deviation from the Kardar–Parisi–Zhang universality class, model valid for only one kind of deposited particles. The study also shows that when the deposition of particles with less active bonds occurs more frequently the voids under the surface become relevant. However, the increase in overhang/voids processes under the moving interface does not strengthen greately the local surface gradient. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

The growth of surfaces and interfaces is a subject of considerable current interest [1,2]. The microscopic mechanisms of such kind of problems were not extensively studied in the past except for the cases of one kind of deposited species. However, due to the demand of modern technologies, it is common to find a growth of binary or more types of deposited components. Moreover, the study of this problem is of great importance due to the fact that the growth process may belong to a new universality class [3–5]. The kinetic roughening upon starting from an initially flat substrate is a common phenomena in the growth of a surface as well as the existence of the dynamic scaling [1]. Defining the surface width $W(L,t) = \sqrt{\frac{1}{L^{d-1}} \sum_r [h(r,t) - \overline{h(t)}]^2}$, 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

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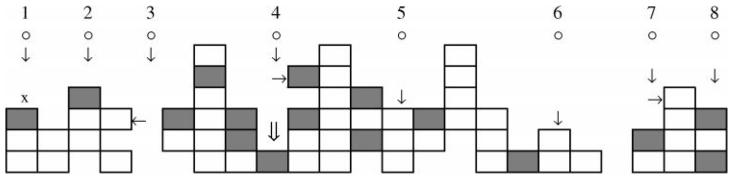

Fig. 1. A cross-sectional piece of the aggregate.

average height at time t and $(d-1)$ is the substrate dimension, the scaling law [1] is given by $W(L,t)=L^{\alpha}f(t/L^{z})$ where α, β and $z=\alpha/\beta$ are roughness, growth and dynamic exponents, respectively. The scaling function $f(x)=x^{\beta}$ for $x \ll 1$ and $f(x)=constant$ for $x \gg 1$. Previous studies show that for $d>2$ there is still disagreement over the values of the exponents as well as the universality of the various surface growth models [2]. Therefore, for $d>2$, the study of discrete models may provide new insight into the dynamics of the surface growth. In addition, there may exist a new universal behaviour especially in the case of growth of binary mixtures where little is known about kinetic roughening [3–5]. Several studies for the growth of binary mixtures have been made in the context of the ballistic deposition (BD) model where voids/overhang process is relevant [3,4,7]. Here, we propose to study further the BD model in $2+1$ dimensions for two species. So, we focus on how the interaction between the two different particles affects the kinetics of growth and the morphology.

2. Model

We propose a model adequate to describe reactions which take place on the growing surface of materials. It represents the surface growth of a material with low concentration of impurities. Furthermore, it describes the deposition of two kinds of particles with different attractive forces. The growth process, 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 Fig. 1. The white squares represent the aggregated particles of type A and dark squares represent those of type C. Circles denote the incoming particles. The path of the fallen particle is shown by the arrows. The deposition occurs as follows: a particle of type A will stick to the first particle A or C that meet, either at the top of the chosen column (particles 1, 2, 5, 6 and 8) or sideways (paricles 3, 4 and 7). When the incoming particle is of type C, it sticks to the top of the chosen column if the latter contains particle A (particles 5 and 6) or on one of the neighbouring sites higher by one step if there is a particle of type A (particle 8), or it is discarded if it finds a particle C (particle 1). When the chosen column is lower than its neighbours, C will stick laterally if it finds a particle A (particles 3 and 7) or it will diffuse downwards until it finds a particle of type A (particle 4, double arrow).

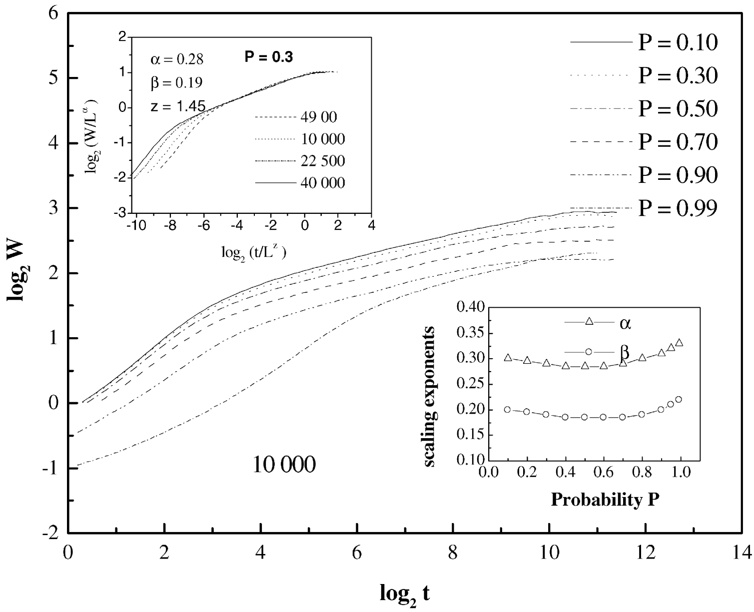

Fig. 2. log–log plot of time versus surface width. The upper inset shows the extraction of the exponents for $P = 0.3$. The lower inset shows the values of the exponents versus the probability.

3. Results

The aggregation occurs in the Z direction with periodic boundary conditions in the X and Y directions on a square lattice. Statistical average is obtained over 500 independent simulations for each parameter. Fig. 2 shows a log–log plot of the surface width W as a function of time (number of the deposited layers) for different values of the probability P and fixed system size $L^2 = 10\,000$. The surface width always decreases and shifts to the right as the probability P increases except for $P = 0.99$. This kinetic is different from that in previous work [3,4] where, we found a rapid increase in the surface width after a certain value of $P = P_c = 0.5$ and the model no longer belong to the KPZ universality [6]. We argue that the change of kinetics in the present case is due to the interactions between the different deposited particles, where particle C is no longer completely inactive. The upper inset of Fig. 2 shows the values of the exponents determined for $P = 0.3$ while in the lower inset the values of the exponents α and β are plotted versus the different values of the probability P. It is well known that the BD model for one kind of deposited particles follows the KPZ universality. However, the values of the exponents show that, the scaling law of the KPZ, where $\alpha + \alpha/\beta \neq 2$, is violated by 10 to 14% for all values of the probability P, while the error in calculating the exponents is roughly 3%. In comparison to the model in Refs. [3,4], the values of the exponents here are completely different from those calculated in the previous model. The exponent β does not increase very rapidly

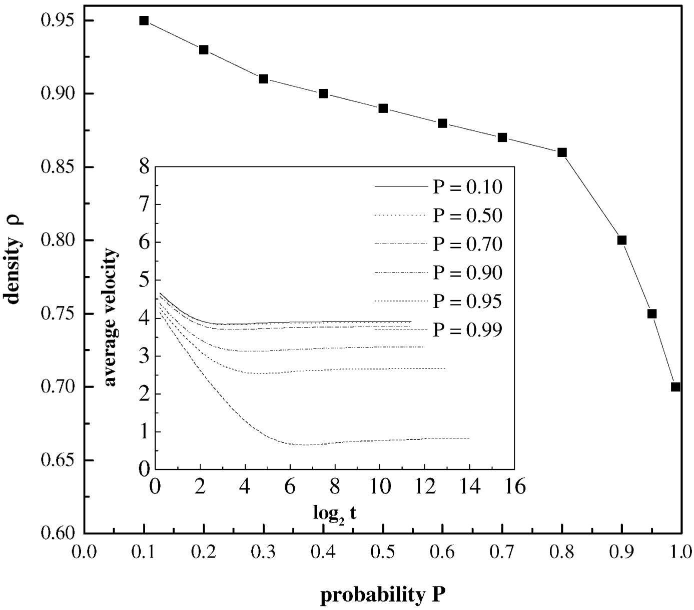

Fig. 3. The density ρ versus probability P. The inset shows the average velocity as a function for time for different values of P.

with P which indicates that the fluctuations in height are not so strong. This supports the argument that the interaction between the deposited particles and the presence of the inactive particles over the surface were responsible for the different kinetic behaviours in the old case. It is known that when voids/overhang processes become dominant, the surface width grows faster [2] since it increases the nonlinear term $(\nabla h)^2$ in the KPZ equation. However, in the old model the rapid increase of the surface width and high values of the exponent β for $P > P_c$ are more related to the nonlocal growth that arises due to the formation of inactive clusters over the surface than to the formation of voids below the surface, since some sites capture most of the incoming flux and grow faster than others. The interface was driven to grow having a high value of β and it saturates earlier in time with a higher value. According to the values of β in this work we suggest that the effect of voids/overhang on the growth rate may start when the density of the aggregate ρ reaches a value lower than a critical ρ_c (more overhang/voids processes) or it may not have a strong effect. Fig. 3 shows the density $\rho = N/\bar{h}L^2$ plotted versus the probability P. It is clear from the figure that the density decreases as P increases. This figure indicates clearly that as P increases more voids are formed while the interface moves. However, the decrease in the density does not affect the kinetics as strong as it is affected in the previous work of Ref. [4] supporting the above argument. In order to enhance the above arguments, we have plotted the velocity of the growth of the interface versus time for different values of P. As shown in the inset of Fig. 3 as P increases the velocity decreases although the overhang/voids processes occur more as P increases. This means that the overhang/voids processes do not reach a value such that the local gradient increases enough to affect the growth rate. This is evident from the fact that the velocity does not increase at intermediate times until saturation [3,4].

4. Conclusion

We have studied the kinetics and morphology of the surface growth BD model for two species in $2+1$ dimensions. We found that the kinetics have a different behaviour than that in Refs. [3,4] due to the allowance of more interaction between the deposited particles. We have also found that the density ρ of the aggregation does not become as low as in the previous case, hence the effect of voids on the local gradient is limited. This shows that the growth exponent does not increase to a large value which indicates that the fluctuations in height are not as high as those observed before. Also the exponents calculated here suggest that the model in this paper may not belong to the KPZ universality class of the BD model for one kind of particles since the deviation from this universality ranges from 10 to 14%, far above the error of computation. This suggestions can be guaranteed through an extensive study of correlations, which lies outside the scope of this work.

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