Static phase and dynamic scaling in a deposition model with an inactive species

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We extend a previously proposed deposition model with two kinds of particle, considering the restricted solid-on-solid condition. The probability of incidence of particle C (A) is p $(1-p)$. Aggregation is possible if the top of the column of incidence has a nearest neighbor A and if the difference in the heights of neighboring columns does not exceed 1. For any value of $p>0$, the deposit attains some static configuration, in which no deposition attempt is accepted. In $1+1$ dimensions, the interface width has a limiting value $W_s \sim p^{-\eta}$, with $\eta=3/2$, which is confirmed by numerical simulations. The dynamic scaling relation $W_s = p^{-\eta} f(tp^z)$ is obtained in very large substrates, with $z=\eta$.

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I. INTRODUCTION

Statistical growth models of surfaces and interfaces have attracted much attention in the last two decades, motivated by technological applications of thin films and related nanostructures [1–4]. In recent work, models with two types of particle were introduced, in order to represent the effects of different chemical species in deposition processes [5–12]. The competition of different growth mechanisms may lead to crossover of growth exponents and roughening transitions, as observed in many systems with a single species [13–20].

A particularly interesting two-species model was proposed by Wang and Cerdeira [5], which will be called the AC model. In that model, particles A and C are released with probabilities $1-p$ and p, respectively, and aggregation is allowed only if the incident particle encounters a neighboring A at the sticking position (which may be defined by different rules). Thus, particles C represent impurities that block the growth in their neighborhoods. For high p, the surface will be contaminated with this species and the growth process will fail. In previous work, the crossover of growth exponents was studied in the growth regime [5–7].

In the present work, we will consider the restricted solid-on-solid (RSOS) version of the AC model. The RSOS model was introduced by Kim and Kosterlitz in 1989 to describe the growth of thin films in which the height differences between neighboring columns do not exceed a certain limiting value ΔH_{max}. This condition prevents the formation of high local slopes in the film surface [21]; thus it is interesting for the description of deposition processes in which diffusion and desorption mechanisms (not explicitly included in the model) favor the formation of locally smooth surfaces.

The RSOS version of the AC model is defined as follows. At each deposition attempt, an incident particle A or C is chosen with the probabilities $1-p$ and p, respectively. This particle is released above a d-dimensional substrate in a randomly chosen column. The sticking position for the incident particle is the top of the selected column, but aggregation is possible only if both the following conditions are satisfied: (a) the difference in the heights of neighboring columns does not exceed $\Delta H_{max}=1$; (b) the sticking position has a nearest neighbor particle A. If one or both conditions are not satisfied, then the deposition attempt is rejected. Figure 1 illustrates the deposition rules.

Here we will study the model in $d=1$. We will show that a dynamic transition occurs at $p=0$ because any finite flux of particles C will eventually suppress the growth process. Thus, at $p>0$ the model presents a static phase, i.e., the film attains a configuration that cannot continue growing because no deposition attempt can be accepted. The interface width at saturation scales with p with an exponent η that can be exactly obtained. It is also shown that the dynamic exponent of the model is $z=\eta$. The features of this static phase differ from the dynamic nature of the smooth phases of other models with roughening transitions, such as those including competition between adsorption and desorption of adatoms [13–17]. However, there are many important open questions in the field of roughening transitions, such as the exponents' relations [14], thus some results presented here may also be helpful in that context.

The rest of the paper is organized as follows. In Sec. II we present the simulation results and discuss the transition at $p=0$. In Sec. III, we obtain a dynamic scaling relation for the interface width. In Sec. IV we present our conclusions.

II. NUMERICAL SIMULATIONS AND THE DYNAMICAL TRANSITION

The main quantity of interest in deposition models is the interface width W of the deposit. In a surface of length L (L^d columns), at time t, W is defined as

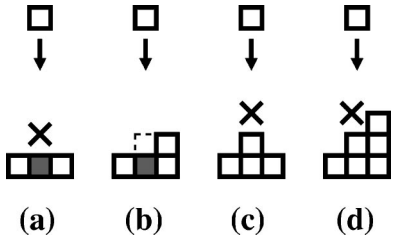

FIG. 1. Examples of application of the deposition rules of the RSOS version of the AC model. Open squares represent particles A and filled squares represent particles C. In (a), the aggregation attempt is not accepted because there is no neighboring A at the top of the column. In (b), this neighbor is present (the dashed square indicates the sticking position). In (c) and (d), the aggregation attempt is not accepted because it would violate the RSOS condition.

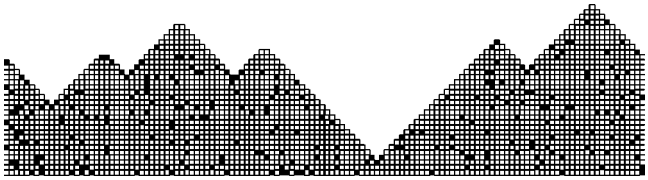

FIG. 2. Example of a final static deposit for $p=0.1$ and $L=128$.

$$W(L,t)=\left[\left\langle \frac{1}{L^d}\sum_i (h_i-\overline{h})^2\right\rangle\right]^{1/2}, \tag{1}$$

where h_i is the height of column i, the overbar on $\overline{h}$ denotes a spatial average, and the angular brackets denote a configurational average, i.e., an average over many realizations of the noise.

In the pure RSOS model ($p=0$), W obeys the dynamic scaling relation

$$W\approx L^{\alpha} f(tL^{-z}). \tag{2}$$

The exponents α and z are consistent with the Kardar-Parisi-Zhang (KPZ) theory [22], which provides a hydrodynamic description of kinetic surface roughening. In $d=1$, the KPZ equation gives the exact values $\alpha=1/2$ and $z=3/2$ [22].

We simulated the RSOS version of the AC model for several values of p, most of them between $p=0.003$ and $p=0.02$. Substrates of lengths L from $L=256$ to $L=65\,536$ were considered, with periodic boundaries. During the simulations, the time was measured as the number of deposition attempts per column; thus one time unit corresponds to L deposition attempts (accepted or not). For each p and L, we generated 10 sets with 10^3 different deposits in each, and calculated error bars from the fluctuations of the average values of the different sets.

In all cases, the growth process fails at sufficiently long times, when the interface width attains a limiting value $W_s(p,L)$. In Fig. 2 we show a deposit for $p=0.1$ and $L=128$ in which no aggregation is possible. Notice that the deposit is faceted, consisting of a set of droplets of triangular shape. In the valleys of the deposit, there are triplets of particles C with the structure shown in Fig. 3. Eventually, groups of four or more particles C may create such valleys, but they are much less probable than the triplets if p is small. These structures and the RSOS condition are responsible for the suppression of the growth process.

For any $p>0$, the saturation width W_s converges to a finite value with vanishing $1/L$ corrections. This contrasts with the behavior of moving phases, where the saturation width diverges as L^{α}, with $\alpha>0$ [Eq. (2)]. Extrapolations to $L\to\infty$ give $W_s(p,\infty)$ and the average saturation height $H_s(p,\infty)$. The errors in $H_s(p,\infty)$ are usually lower than 1%, and the errors in $W_s(p,\infty)$ are nearly 10%.

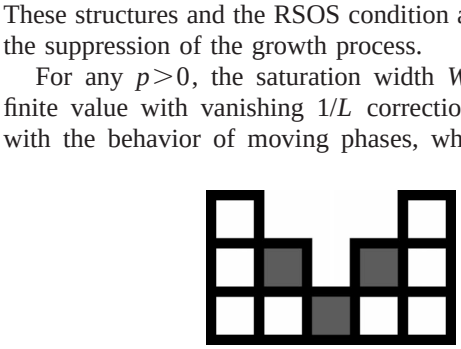

FIG. 3. Triplet of particles C (filled squares), which occupies most valleys of the static deposits, surrounded by A particles.

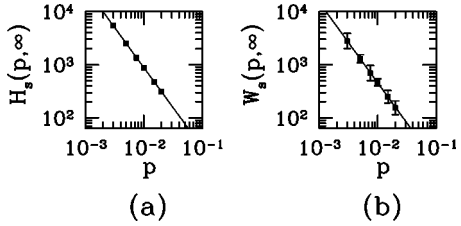

FIG. 4. (a) Saturation height $H_s(p,\infty)$ in very large substrates versus probability p of incidence of particles C; (b) saturation width $W_s(p,\infty)$ versus probability p. Solid lines are least squares fits.

In Fig. 4(a) we plot $\log_{10}H_s(p,\infty)$ vs $\log_{10}p$ and in Fig. 4(b) we plot $\log_{10}W_s(p,\infty)$ vs $\log_{10}p$. These quantities scale as

$$W_s(p,\infty)\sim H_s(p,\infty)\sim p^{-\eta}, \tag{3}$$

with $\eta=1.509$ obtained from the least squares fit of the H_s data, and $\eta=1.515$ obtained from the fit of the W_s data. These relations show that the growth process will actually fail for any $p>0$.

Our numerical results suggest the exact value $\eta=3/2$, which can be obtained using scaling arguments, as follows. The onset of triplets of particles C is responsible for the suppression of the growth process, and each blocking configuration has probability of order p^3. A mound of triangular shape (between valleys containing triplets of C) has a height of order W_s; thus the number of particles A in the mound is of order W_s^2. Thus, for small $p, W_s^2\sim 1/p^3$, giving $\eta=3/2$.

III. DYNAMIC SCALING

The weak finite-size effects for large L suggest that a dynamic scaling relation in the static phase must be expressed only in terms of the probability p and the time t, while terms involving the length L will be (vanishing) corrections to scaling.

For very large L, we propose the scaling relation

$$W\approx p^{-\eta} f(t/\tau), \quad \tau\sim p^{-z}, \tag{4}$$

where τ is a characteristic time for the onset of correlations between the C triplets, and z is a dynamic exponent. τ is a measure of the number of layers of the deposit when these correlations appear; thus we expect that $\tau\sim H_s$. Since H_s also scales with the exponent η [Eq. (3)], we obtain

$$z=\eta=\frac{3}{2}. \tag{5}$$

In order to test relation (5) with the above exponents, we plot Wp^{η} versus tp^z in Fig. 5, considering three values of p: $p=0.005$, $p=0.01$, and $p=0.02$. Those data were obtained in substrates with $L=65\,536$, which are sufficiently large to

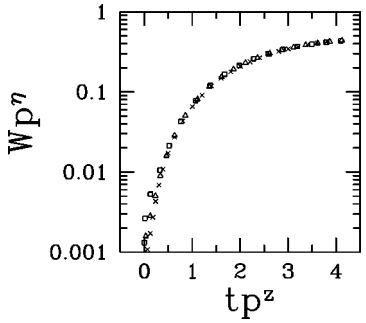

FIG. 5. Log-linear plot of Wp^{η} versus tp^{z}, with $\eta=z=3/2$, using data obtained in substrates with $L=65\,536$ and probabilities $p=0.02$ (squares), $p=0.01$ (triangles), and $p=0.005$ (crosses).

minimize finite-size effects. The good data collapse in Fig. 5 confirms the validity of the scaling relation (5).

Finally, it is interesting to notice the divergence of the data for different p at $t \lesssim 0.5p^{-z}$, as shown in Fig. 5. At very short times, we expect that the interface width scales as in the pure RSOS model, with no dependence on p, because the effects of C particles are negligible. Then the pure RSOS model regime, in which the width increases with time as $t^{1/3}$, becomes just a transient region for any $p>0$.

IV. DISCUSSION AND CONCLUSION

We studied a deposition model with two types of particle A and C, in which incident particles can stick only at positions that have a neighboring A and if the RSOS condition is satisfied. For any flux of particles C, the growth eventually fails, due to the RSOS condition and the formation of triplets of C. The saturation width W_s is obtained in the static final configurations in sufficiently large substrates. Scaling arguments show that it scales as $W_s \sim p^{-3/2}$ for small p, and this result is confirmed by numerical simulations. The interface width W obeys a dynamic scaling relation involving the probability p and the deposition time t [Eq. (4)].

This model represents some growth mechanisms in the presence of impurities. As proposed in Ref. [5], it may describe the effects of the deposition of an active particle B that reacts with a previously aggregated particle A and forms the inactive particle C. In the present RSOS version, small concentrations of the impurity may suppress the growth process, with the inactive particles forming the pinning centers. The blocking configurations depend on the particular model considered (for instance, they will change for different ΔH_{max}), and the value of the exponent η depends on the number of particles C in those configurations. In a deposit with simple cubic lattice structure (which is more suitable for real applications) and $\Delta H_{max}=1$, configurations with five particles C will form the pinning centers, and the supression of the growth process will also be observed.

Previous work has also shown transitions from a moving phase to a smooth phase [13,14,16,17]. In the moving phases, as the critical points are approached, the growth velocities continuously decrease to zero. The smooth or anchored phases correspond to the active (ordered) phases of other processes, such as directed percolation. The present model has many differences from those. First, the growth velocity changes discontinuously from a finite value at $p=0$ (pure RSOS model) to zero at $p>0$. Furthermore, if we consider the order parameters M_i defined in Ref. [14] ($i=1,2,\ldots$), we obtain $M_i=0$ in the static phase, since there is no preferential level for the pinning centers (see Fig. 2). Thus, this phase is not ordered in that sense. Despite those differences, we expect that the analysis that led to the dynamic scaling relation (4) may be extended to other systems and may be useful to predict relations between growth exponents.

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