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Roughness scaling and sensitivity to initial conditions in a symmetric restricted ballistic deposition model

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Abstract. In this work, we introduce a restricted ballistic deposition model with symmetric growth rules that favors the formation of local finite slopes. It is the simplest model which, even without including a diffusive relaxation mode of the interface, leads to a macroscopic groove instability. By employing a finite-size scaling of numerical simulation data, we determine the scaling behavior of the surface structure grown over a one-dimensional substrate of linear size L. We found that the surface profile develops a macroscopic groove with the asymptotic surface width scaling as $w_{\rm sat} \propto L^{\alpha}$, with $\alpha = 1$. The early-time dynamics is governed by the scaling law $w \propto t^{\beta}$, with $\beta = 1/2$. We further investigate the sensitivity to initial conditions of the present model by applying damage spreading techniques. We find that the early-time distance between two initially close surface configurations grows in a ballistic fashion as $D \propto t$, but a slower Brownian-like scaling ($D \propto t^{1/2}$) sets up for evolution times much larger than a characteristic time scale $t_{\times} \propto L^2$.

PACS. 05.70.Np Interface and surface thermodynamics – 68.35.Ct Interface structure and roughness – 81.15.Aa Theory and models of film growth

1 Introduction

The dynamics of growing surfaces [1] has been a subject of increasing interest in material science impelled by ongoing developments on techniques such as vapor deposition, molecular-beam-epitaxy and sputtering. Very recent advances in the field of ballistic deposition processes [2–9] and the general problem of surface growth kinetics and fractal scaling [10–17] have further broadened the relevance of such developments. Several stochastic non-equilibrium models have been proposed to describe the surface morphology and evolution resulting from distinct growth processes. It has been well established that the dominant relaxation mode plays an important role in determining the scaling behavior of surface roughening [18].

The growth dynamics is well described by the Kardar-Parisi-Zhang [19] equation when desorption is the relevant process governing the surface relaxation. Dynamic renormalization group analyses of the KPZ equation have shown that the rms fluctuation in the surface height, known as the surface width w, is described by the scaling relation

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

where L is the linear dimension of the substrate, with $\alpha = 1/2$ and $z = 3/2$ in the case of a one-dimensional substrate [19]. The surface roughness width w saturates as $w_{\rm sat} \propto L^{\alpha}$, but exhibits an initial power law increase with time according to $w \propto t^{\beta}$, with $\beta = \alpha/z$. Ballistic deposition (BD) is the simplest lattice model which captures the essence of the lateral surface growth (*e.g.*, in growth processes with desorption). Numerical simulations have shown that the BD model indeed belongs to the same universality class as the KPZ equation [1].

In contrast, surface diffusion is the relevant relaxation mode in film growth techniques such as molecular beam epitaxy and vapor deposition [20]. Several stochastic discrete on-lattice models and continuous differential equations have been proposed for describing these processes. Some of these models exhibit a breakdown of translational invariance. The surface develops a macroscopic groove as a consequence of an intrinsic instability favoring the creation of large slopes in the interface which are limited only by the periodic boundary conditions [18,20]. For sputtering, instabilities can lead similarly to the formation of ripples [21–23].

Constraints imposed on the surface relaxation modes can usually modify the universality class governing the temporal evolution of the surface width. In particular, Park *et al.* introduced a new ballistic deposition model on which local height differences are restricted to be positive or zero [24]. For an initially asymmetric interface, with all local differences being non-negative, they showed that the surface width within this restricted model has an asymptotic width characterized by the same roughness

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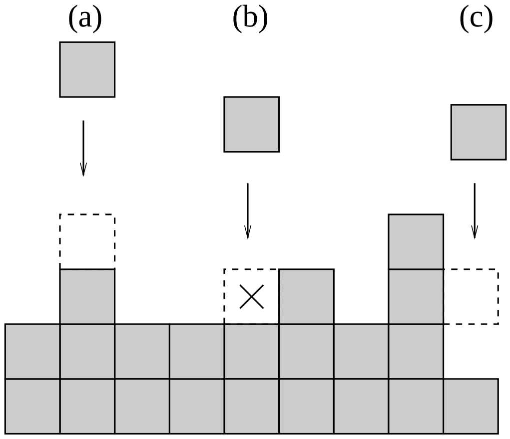

Fig. 1. (a) Example of a deposition process permitted in both BD as well as SRBD. (b) Example of a process permitted in BD that is prohibited in SRBD. This restriction kills very many potential deposition processes. (c) Example of a second-layer lateral deposition process that is permitted in SRBD but which does not occur in BD.

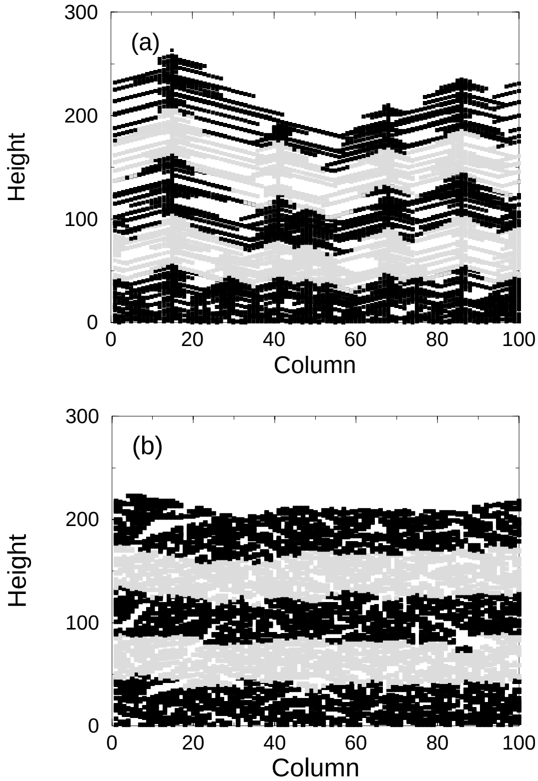

Fig. 2. (a) Symmetric restricted ballistic deposition surface growth for $L = 100$, in contrast to (b) classic ballistic deposition, for 2×10^4 particles in groups of 4×10^3.

exponent α of the unrestricted model, *i.e.*, $\alpha = \alpha_{\mathrm{KPZ}}$. However, the dynamic exponent β was found to be given by $\beta = \beta_{\mathrm{KPZ}}/(1 - \beta_{\mathrm{KPZ}})$.

In this work, we introduce a new symmetric restricted ballistic deposition model. The model allows for lateral growth and favors the formation of finite local slopes. We will show that, even in the absence of particle diffusion, an initially smooth surface exhibits a translational symmetry-breaking, developing a groovy asymptotic profile. By employing a finite-size scaling of numerical data, we obtain the dynamic scaling exponents. Further, we characterize the sensitivity to initial conditions on this model through a damage spreading analysis.

2 Symmetric restricted ballistic deposition model – SRBD

In what follows, we consider a ballistic deposition (BD) model for the growth of an interface over a one-dimensional substrate. In this model, particles are released from randomly chosen positions above the surface, located at a distance larger than the maximum height of the interface (Fig. 1a). In the simplest version of the model, each particle follows a straight vertical trajectory until it reaches the surface. In classic BD, the particle sticks to the first particle it encounters in the surface, either on top (vertical growth) or laterally (horizontal growth). Here we introduce a restricted growth model by imposing the condition that the lateral growth take place only by the adsorption of the particle on the lower diagonal (see Fig. 1c); if the corresponding site is already occupied, the particle does not attach on the surface. Therefore, within the above growth rules, the dynamic processes in which the growing columns' heights equal their nearest neighbors' are rejected (Fig. 1b).

The deposited particles form a cluster (or aggregate) with a very characteristic geometry. Figure 2a shows the structure produced by the model after the deposition of 2×10^4 particles — in comparison to the structure produced by the standard ballistic model in Figure 2b. These figures highlight the position of the interface at successive intervals of 4×10^3 deposited particles, so that the growth process can be followed qualitatively. In the SRBD an initially flat interface roughens at early times but gradually develops local grooves. After a long deposition period, a single groove profile sets up as in MBE models with particle diffusion. The position of the dominant groove randomly changes from one experiment to another reflecting the breakdown of the translational invariance.

In order to describe quantitatively the interface growth in the SRBD model, we computed the interface width w that characterizes the roughness of the interface. It is defined as the rms fluctuation in the height,

$$w(L,t) \equiv \sqrt{\frac{1}{L}\sum_{i=1}^{L}[h(i,t) - \bar{h}(t)]^2}, \qquad (2)$$

where $h(i,t)$ is the height of column i at time t and $\bar{h}(t)$ is the mean height of the surface at time t.

In all our simulations, the growth starts from a horizontal line with periodic boundary conditions; the interface at time zero is simply a straight line, with zero width.

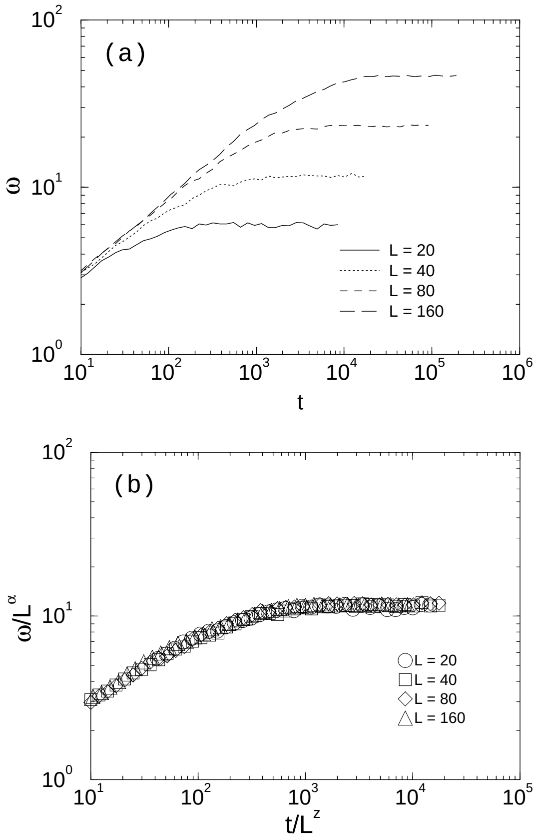

Fig. 3. Time evolution of (a) the surface width for various L and (b) after rescaling. Here, $\alpha = 1$ and $z = 2$. The configurational average was carried out over 800 surfaces. Time here is measured in lattice sweeps, *i.e.* L particles are dropped per unit time.

As deposition occurs, the interface gradually roughens as already evidenced in Figure 2a.

3 Scaling behavior in the SRBD model

A typical plot of the time evolution of the surface width in the SRBD has two regions separated by a 'crossover' time $t_\times$ as in the standard BD model (see Fig. 3a). Initially, the width increases as a power of time,

$$w(L,t) \sim t^\beta \qquad [t \ll t_\times]. \tag{3}$$

The growth exponent β characterizes the time-dependent dynamics of the roughening process. The power-law increase in width does not continue indefinitely, but is followed by a saturation regime (the horizontal region of Fig. 3a) during which the width reaches a saturation value, w_{sat}. In Figure 3a, four different curves correspond to the time evolution of the width obtained by simulating systems with four different sizes L. As L increases, the saturation width, w_{sat}, increases as well, and the dependence also follows a power law,

$$w_{\text{sat}}(L) \sim L^\alpha \qquad [t \gg t_\times]. \tag{4}$$

The roughness exponent α characterizes the roughness of the saturated interface. The crossover time $t_\times$ (sometimes called saturation time) at which the interface crosses over from the behavior of equation (3) to that of equation (4) depends on the system size,

$$t_\times \sim L^z, \tag{5}$$

where $z = \alpha/\beta$ is the dynamic exponent.

The above exponents can be estimated by employing a data collapse of the finite size data onto a universal curve. $w(L,t)/w_{\text{sat}}(L)$ is a function of $t/t_\times$ only, *i.e.*,

$$\frac{w(L,t)}{w_{\text{sat}}(L)} \sim f\left(\frac{t}{t_\times}\right), \tag{6}$$

where $f(u)$ is called a scaling function. Replacing w_{sat} and $t_\times$ by their scaling forms, we obtain the Family-Vicsek scaling relation (Eq. (1)).

The general form of the scaling function $f(u)$ can be seen from Figure 3a. There are two different scaling regimes depending on $u \equiv t/t_\times$. For small u, the scaling function increases as a power law. As $t \longrightarrow \infty$, the width saturates. In this limit, $f(u) = \text{const}$.

We test the validity of the scaling relation (Eq. (1)) numerically by re-plotting the data of Figure 3a. By plotting on the horizontal axis t/L^z, and on the vertical $w(L,t)/L^\alpha$, the curves from different linear sizes collapse onto the scaling function $f(u)$ once the proper exponents are used. The rescaled curves are shown in Figure 3b, and the data collapse found indeed supports the scaling hypothesis. The scaling exponents found for the SRBD model are $\alpha = 1$ and $z = 2$ ($\beta = \alpha/z = 1/2$). Note that the growth exponent β of the SRBD model is the same as that found for the RBD model [24] once these exhibit the same time scales. On the other hand, the roughness exponent α is quite different; its value $\alpha = 1$ indicates that the SRBD model is indeed at the threshold of instability for the generation of large local slopes.

We now briefly discuss the deeper mathematical reasons underlying the extremely large values of $\alpha \gg 1/2$ observed in the SRBD model. Usually such behavior arises from diffusion, but this model inherently lacks diffusion, hence the instability arises *purely* from the dynamical growth rules. By allowing lateral growth *only* on the second layer rather in the same layer, the model forces all lateral growth to lead to a local surface slope of 1. At the same time, vertical growth is prohibited whenever it leads to a reduction of the local slope. Hence, this model very quickly generates long-range correlations along the surface, tending ultimately to a single sloping surface. The SRBD model is important because it is the simplest which, without including a diffusive relaxation mode of the interface, leads to macroscopic grooves with $\alpha = 1$.

4 Damage spreading in the SRBD model

The damage spreading technique is an important tool for investigating the sensitivity to initial conditions in nonlinear dynamical systems [25–29]. The important measurable quantity in this technique is the Hamming distance

D, defined as the difference between two configurations of the system evolving under identical external noise and whose initial state differs only by a very small perturbation. It has been previously used in various discrete-growth models to explore the relation between the surface correlation length and the propagation distance of the perturbation [30].

Here, we follow the temporal evolution of two interfaces A and B. The initial condition of system A is a flat interface with $h^{\rm A}(i,0) = 0$ for all positions i. The initial condition of system B differs from that of system A by a small bump at a randomly chosen site i_0, *i.e.*, $h^{\rm B}(i,0) = \delta_{i,i_0}$. Then both interfaces are evolved under identical dynamical rules of the SRBD model. The same sequence of random numbers is used during the growth of both surfaces to simulate a common external noise. We define the Hamming distance as

$$D(t) = \frac{1}{L}\sum_{i=1}^{L} |h^{\rm A}(i,t) - h^{\rm B}(i,t)|. \qquad (7)$$

In the standard BD model, the dynamic scaling behavior of the Hamming distance can be directly related to the proper scaling of the surface width. In the BD model the maximum difference between the heights of columns in system A and B is $\max|h^{\rm A}(i,t) - h^{\rm B}(i,t)| = 1$. Therefore the Hamming distance should saturate at a maximum value $D(t \to \infty) = 1$. At early times the set of damaged columns is compact and its size scales as the correlation length, thus giving rise to a power-law increase of the Hamming distance as $D(t) \propto t^{1/z}$ [24].

The present SRBD model exhibits a breakdown of translational invariance. As a consequence, the surface develops a groove whose peak randomly changes from one experiment to the other. Therefore, even two initially close interface configurations will become asymptotically uncorrelated. Following this reasoning, the Hamming distance is expected not to saturate but to grow in a Brownian fashion as $D(t) \propto t^{1/2}$ after a transient time of order $t_\times$. In Figure 4a we plot $D(t)/t^{1/2}$ *versus* t for distinct lateral sizes L which exhibit the above trend. These curves can also be collapsed onto a universal curve by properly rescaling the time axis as shown in Figure 4b. Once the Brownian divergence of the two configurations is taken into account, the sensitivity to initial conditions at early times can be related to the correlation length exponent as $D(t)/t^{1/2} \propto t^{1/z}$. Therefore the Hamming distance has a crossover from a fast ballistic-like behavior $D(t) \propto t^{1/2+1/z}$ for $t \ll t_\times$ to a slower Brownian divergence $D(t) \propto t^{1/2}$, for $t \gg t_\times$.

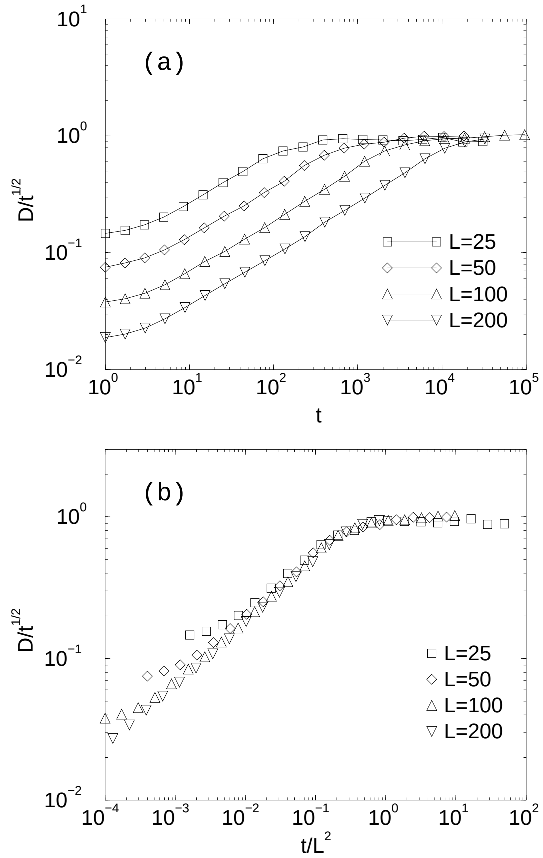

Fig. 4. (a) Time evolution of Hamming distance and (b) Hamming distance as a function of time rescaled by L^2. For very small times, note the breakdown in scaling. The configurational average was carried out over 800 surfaces. The different curves correspond to simulations for different system sizes L.

5 Conclusions

In this work, we have introduced a symmetric restricted ballistic deposition model which develops a groove instability in the absence of particle diffusion. The model is a variant of the standard ballistic deposition. It allows for lateral growth only along the lower diagonal of the first site on the interface found by an ejected particle. However, it rejects processes which would imply in the overtaking of a local maximum, thus favoring the formation of finite local slopes.

We have employed a finite-size scaling analysis of data from the surface width and computed the scaling exponents governing the interface roughness. We have found that the roughness exponent $\alpha = 1$ as a signature that this model is in the threshold of instability to the developing of large local slopes. Indeed, the asymptotic profile resulting from the SRBD dynamical rules exhibits a breakdown of translational invariance and develops a groove with unit slope. The growth exponent was found to be $\beta = 1/2$, in agreement with the result for the RBD model which exhibits the same time scale [24].

Further, we have investigated the sensitivity to initial conditions of the SRBD model by using the damage spreading technique. We have found that the distance between two initially close interface configurations grows at early times in a ballistic fashion $D(t) \propto t$ and therefore faster than the correlation length $\xi(t) \propto t^{1/z}$ ($z = \alpha/\beta = 2$). In this sense, the sensitivity to initial conditions of the SRBD model is similar to the one reported for the larger curvature model [24]. For systems of finite size, the configurations become uncorrelated after a crossover time $t_\times \propto L^z$, and a slower Brownian divergence of the configurations sets up.

In summary, we report the fundamentally relevant scaling exponents related to the SRBD model. This model is the simplest one which, without including a diffusive relaxation mode of the interface, exhibits a macroscopic groove instability. There is great potential for the the model to be used as a prototype to study the development of the grooved phase and for investigating groove instability in surface growth models.

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