

Restricted curvature model with suppression of extremal height

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A discrete growth model with a restricted curvature constraint is investigated by measuring both the surface width and the height difference correlation function. In our model, where an extremal height is suppressed, the surface width W shows the roughness exponent $\alpha \approx 0.561$ and the dynamics exponent $z \approx 1.69$ in one substrate dimension. However the correlation function has an unusual scaling behavior and produces different wandering exponent $\alpha' \approx 1.33$ and its dynamic exponent $z' \approx 4$. The discrepancy is due to the fact that the correlation length increases with a power law $t^{1/z'}$ until it reaches the value proportional to L^δ at time $t_s \sim L^z$, where L is the system size and δ is the “window exponent” satisfying the relation $\delta = z/z' = \alpha/\alpha'$. δ is a new exponent to characterize the window size of the system.

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Kinetic roughening of interfaces has been intensively studied [1–4] for the last decade or so with the use of both analytical continuum growth equations and discrete atomistic numerical simulations. Various dynamic growth universality classes have been identified for growth models with each universality class corresponding to a particular continuum growth equation for the coarse-grained height variable $h(x, t)$, which describes the growing interface as a function of the lateral surface coordinate x and growth time t . Substantial theoretical efforts have gone into classifying the universality classes of discrete growth models [1–4]. This is typically done numerically in a rather *ad hoc* manner by measuring the simulated critical growth exponents of the discrete models.

An interesting quantity of the dynamic growth process is the kinetically rough self-affine surface structure. Most recent work concentrates on studying the surface structure of the growth models, especially on determining the dynamical critical exponents governing the surface fluctuations. The dynamic scaling hypothesis is that in a finite system of lateral size L , the variation or the mean square fluctuation W^2 of the surface height starting from a flat substrate scales as [5,6]

$$W^2(L, t) \sim L^{2\alpha} f_w(t/L^z), \quad (1)$$

where α and z are the “roughness” and “dynamic” exponents and the scaling function $f_w(x)$ is $x^{2\beta}$ with the “growth exponent” $\beta = \alpha/z$ for $x \ll 1$ and is constant for $x \gg 1$.

In addition to the surface width, there is another interesting quantity called the correlation function, which involves the square of the height difference in distance r [7,8],

$$G(r, t) = \langle [h(x, t) - h(x + r, t)]^2 \rangle. \quad (2)$$

It also shows a scaling behavior

$$G(r, t) \sim r^{2\alpha'} g(r/\xi(t)) \quad (3)$$

with the wandering exponent α' and a correlation length $\xi \sim t^{1/z'}$. The correlation dynamic exponent z' governs the correlation length along the surface. For conventional mod-

els, the correlation length ξ grows as $t^{1/z'}$ at the beginning and eventually saturates at the system size L [9];

$$\xi(L, t) \sim L g_\xi\left(\frac{t^{1/z'}}{L}\right) \sim \begin{cases} t^{1/z'} & \text{for } t^{1/z'} \ll L \\ L & \text{for } t^{1/z'} \gg L, \end{cases} \quad (4)$$

where the scaling form $g_\xi(x)$ is x for $x \ll 1$ and is constant for $x \gg 1$. In this case, it is easy to prove that the values of α' and z' are the same as α and z of the surface width, respectively.

Here we introduce a new model named “suppressed restricted curvature” (SRC) model which shows $z' \neq z$. This is a discrete growth model in restricted curvature (RC) constraint where an extremal height is suppressed. For completeness, we explain the RC model [10] briefly. The growth rule of the equilibrium RC model is to randomly select a site on a one-dimensional (1D) substrate and then to take a random action between deposition or evaporation (within the solid on solid condition) with equal probability, provided that the restriction on the local curvature $|\nabla^2 h| = |h(x+1) + h(x-1) - 2h(x)| \leq 2$ is obeyed at both the selected site and the nearest neighbor sites. If this RC condition is not satisfied, the corresponding deposition or evaporation event is forbidden. (No relaxation or hopping of the deposited atom is allowed in the model.) Thus, the model is analogous to the restricted solid on solid model [7,8] except that the restriction is on the local curvature $\nabla^2 h$ rather than on the height difference. The RC model is believed to belong to the fourth-order continuum linear equation

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = -\nabla^4 h(\mathbf{x}, t) + \eta(\mathbf{x}, t), \quad (5)$$

where the $\eta(\mathbf{x}, t)$ is an uncorrelated Gaussian noise. This equation can be solved exactly giving $\alpha = \alpha' = 3/2$ and $z = z' = 4$, i.e., $\beta = 3/8$ [10,11].

The rule for the SRC model is the same as that of the RC model except a suppression for the global extremal heights. All possible 1D RC configurations are allowed, but the global maximum and minimum sites are biased to move to the

direction of reducing the surface width. This model may mimic the motion of a step in a vicinal surface where its motion is bounded in two neighboring steps. In equilibrium, these dynamics produce an ensemble of RC surfaces with an exponentially decreasing weight for increasing surface width. We obtain the roughness exponent $\alpha \approx 0.561$ and its dynamic exponent $z \approx 1.69$ by measuring surface width $W(\alpha' \approx 1.33, L, t)$. However, the height correlation function $G(r, t)$ shows different scaling exponents $\alpha' \approx 1.33$ and $z' \approx 4$. The implication of our observation is that the correlation length ξ grows as $t^{1/z'}$ initially and saturates at the value $\xi_s \sim L^\delta$ with $\delta = z/z' \approx 0.423$.

The dynamics and equilibrium properties of our model are studied by Monte Carlo simulations with a Metropolis-type algorithm. Starting from a flat surface, i.e., $h(x, t) = 0$ for all $x = 1, \dots, L$ at $t = 0$, a site is chosen randomly. We try to add or subtract the column height by 1 with the same probability $1/2$. Unless the updated height introduces a new extremal height (new maximum or minimum), the new configuration is accepted as long as it satisfies the RC condition. When it brings a new extremal height, it increases the absolute surface width $W_{abs} = h^{max} - h^{min} + 1$, where h^{max} and h^{min} are the maximum and minimum heights, respectively. In this case, the acceptance probability of the new configuration is reduced by a factor of $p_{out} \leq 1$. The equilibrium partition function of this model is a sum of the weights, $(p_{out})^{W_{abs}}$, over all possible RC surface configurations [12,13]. In our simulation, we choose $p_{out} = 1/2$.

We first measure the mean square surface width $W^2(L, t)$ defined by

$$W^2(L, t) = \overline{\langle [h(t) - \bar{h}(t)]^2 \rangle}, \quad (6)$$

and check the validity of Eq. (1) for our model. Here, \bar{A} and $\langle A \rangle$ represent the spatial and the ensemble averages of A , respectively. With the periodic boundary condition, the finite size effects are rather strong for W in the feasible system sizes. For the models with globally constrained dynamics, simulations on much larger systems are needed when the periodic boundary conditions are applied even to get the roughness and its dynamic exponents. Therefore, we use the free boundary condition (no RC constraint at the boundary) and measure $W(L, t)$.

For the roughness exponent α describing the saturation of the interface fluctuation, we use the relation $W^2(L) \sim L^{2\alpha}$ for the system sizes $L = 32, 64, \dots, 1024$ in the steady state regime $t \gg L^z$. All data fit well with the form of $W^2(L) \sim L^{2\alpha}$. From the least squares fit, we get

$$\alpha = 0.561 \pm 0.005. \quad (7)$$

To determine the growth exponent β , we measure $W^2(t)$ as a function of time for the system of size $L = 2048$. Through the relation $W^2(t) \sim t^{2\beta}$ for early time $t \ll L^z$, we obtain

$$\beta = 0.332 \pm 0.005 \quad (8)$$

and therefore the dynamic exponent

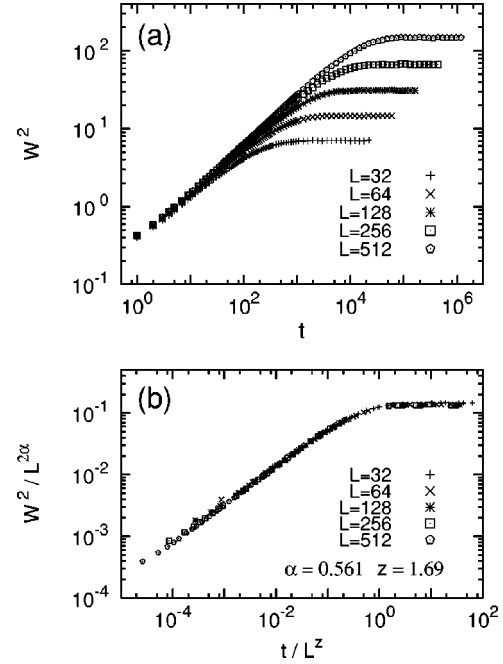


FIG. 1. $W^2(L, t)$ for the systems of sizes $L = 32, 64, \dots, 512$. (a) The plot of $W^2(L, t)$ as a function of t . (b) The scaling plot of $W^2/L^{2\alpha}$ against t/L^z with $\alpha = 0.561$ and $z = 1.69$ ($\beta = 0.332$).

$$z = \alpha/\beta = 1.69 \pm 0.05. \quad (9)$$

Figure 1(a) shows the mean square widths W^2 as a function of t for the systems of sizes $L = 32, 64, \dots, 512$. They increase algebraically initially ($t \ll L^z$ regime) and saturate for $t \gg L^z$ as expected from Eq. (1), where there is a saturation time $t_s \sim L^z$. We check the validity of Eq. (1) by plotting the scaled width $W^2/L^{2\alpha}$ against the scaled time t/L^z . As shown in Fig. 1(b), the scaled data collapse to a single curve with $\alpha = 0.561$ and $z = 1.69$ supporting the scaling behavior of Eq. (1).

We now turn to the height correlation function $G(r, t)$ and consider its scaling behavior of Eq. (3). First, we focus on the short time ($t < L^z$) behavior of the height correlation function for a large system size. Figure 2(a) shows the height correlations $G(r, t)$ for a system of $L = 2048$ at $t = 2, 4, 8, \dots, 1024$. For a given time t , they increase monotonically with r up to the ‘‘correlation length’’ $\xi(t)$ and then remain almost constant for $r > \xi(t)$. The correlation length $\xi(t)$ for a given time t is defined as the distance where $G(r, t)$ becomes saturated. When the scaled height correlations $G(r, t)/r^{2\alpha'}$ are plotted against the scaled distance $r/t^{1/z'}$ with

$$\alpha' \approx 1.33 \quad \text{and} \quad z' \approx 4.0 \quad (10)$$

as shown in Fig. 2(b), the graphs for different times show perfect data collapse indicating the scaling behavior of Eq. (3) with $\xi(t) \sim t^{1/z'}$ for $t \ll L^z$,

$$G(r, t) \sim r^{2\alpha'} g(r/t^{1/z'}). \quad (11)$$

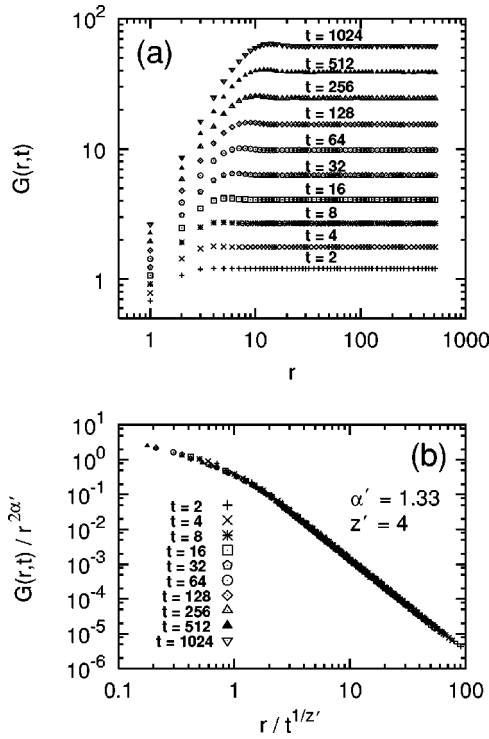


FIG. 2. Height correlation functions $G(r,t)$ for $L=2048$ at intermediate time t . (a) $G(r,t)$ vs r at $t=2, 2^2, \dots, 2^{10}$. (b) The rescaled height correlation function $G(r,t)/r^{2\alpha'}$ against rescaled distance $r/t^{1/z'}$ with $\alpha'=1.33$ and $z'=4$, the data collapse to a single curve supporting Eq. (3).

Note that z' of the SRC model is the same as that of the RC model but α' is not. It seems that the suppression rule of the extremal height mainly affects the wandering exponent α' .

As shown in Fig. 2(a) $G(r,t)$ is independent of r for $r > \xi(t)$. Therefore, we expect

$$g(x) \sim x^{-2\alpha'}, \quad (12)$$

for large x . [Small x behavior of $g(x)$ will be discussed later.] Equations (11) and (12) imply

$$G(r,t) \sim t^{2\alpha'/z'} \quad (13)$$

for $r > \xi(t)$. On the other hand, $G(r,t)$ should be proportional to $t^{2\beta}$ for small t since $W^2(L,t)$ is so. Therefore, we get the relation

$$\beta = \alpha'/z' = \alpha/z. \quad (14)$$

Even though α' and z' are different from α and z , the ratio α'/z' should be same as α/z . Our numerical data of α' and z' satisfy the relation very well.

We then move on to the long-time behavior of $G(r,t)$. We monitor the ‘‘saturate height correlation function’’ $G_s(r) = G(r, t \gg L^z)$ for the system sizes $L=64, 128, \dots, 1024$. As shown in Fig. 3(a), $G_s(r)$ increases only up to a length scale $\xi_s(L)$ and then remains almost constant for $r > \xi_s(L)$. We call $\xi_s(L)$ the ‘‘saturate correlation length’’ or the ‘‘window

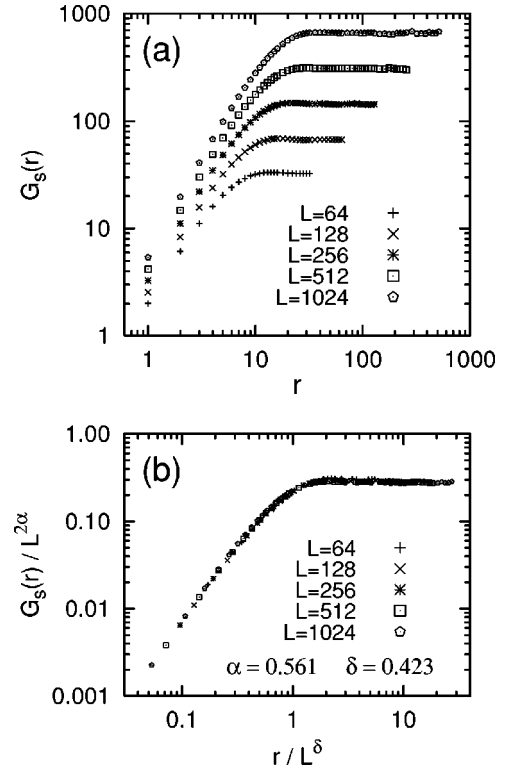


FIG. 3. The saturate height correlation functions. (a) $G_s(r)$ for the systems of sizes $L=64, 128, \dots, 1024$ are shown in log scale. (b) The rescaled height correlation $G_s(r)/L^{2\alpha}$ against rescaled distance r/L^δ with $\alpha=0.561$ and $\delta=0.423$.

size’’ of the system. We assume that $\xi_s(L)$ follow a power-law behavior as a function of L with a new exponent δ called the ‘‘window exponent,’’

$$\xi_s(L) \sim L^\delta, \quad (15)$$

where δ is less than or equal to 1. Since the correlation length increases with a power law $t^{1/z'}$ until it saturates at a value $(t_s)^{1/z'}$ for times $t_s \sim L^z$, we expect

$$\xi_s(L) \sim (t_s)^{1/z'} \sim (L^z)^{1/z'} \sim L^{z/z'}, \quad (16)$$

i.e., $\delta = z/z'$. Since $\alpha/\alpha' = z/z'$ from Eq. (14), we have

$$\delta = \alpha/\alpha' = z/z'. \quad (17)$$

This window exponent δ characterizes the window size of the system and is about 0.423 ($\delta \approx 0.561/1.33 \approx 1.69/4 \approx 0.423$) for our SRC model. With the saturate correlation length of Eq. (15), the height correlation function $G(r,t)$ for late times ($t \gg L^z$) can be written as

$$G_s(r) \sim r^{2\alpha'} g_s(r/L^\delta). \quad (18)$$

When the rescaled saturate height correlations $G_s(r)/r^{2\alpha'}$ are plotted against rescaled distance r/L^δ with $\delta=0.423$, all data collapse to a single curve very well supporting the assumption $\xi_s \sim L^\delta$. The saturate height correlation curve $g_s(x)$

has the same shape as $g(x)$ shown in Fig. 2(b). Above scaling form $G_s(r)$ of Eq. (18) can be reexpressed as

$$G_s(r) \sim L^{2\alpha} \tilde{g}_s(r/L^\delta) \quad (19)$$

with $\tilde{g}_s(x) = x^{2\alpha'} g_s(x)$. Figure 3(b) shows the rescaled saturation height correlations $G_s(r)/L^{2\alpha}$ for the systems of sizes $L=64, 128, \dots, 1024$. When they are plotted against rescaled distance r/L^δ with $\delta=0.423$, all data collapse to a single curve very well implying the scaling form of Eq. (19).

Now the relationship between the roughness and its dynamic exponents (α, z) and the wandering and its dynamic exponents (α', z') are clear. The exponent that describes the time dependence of the correlation length is the wandering dynamic exponent z' [$\xi(t) \sim t^{1/z'}$] but the correlation length increases only up to the saturation correlation length $\xi_s(L)$, which is not proportional to the system size L , but only to L^δ . Therefore, the mean square width for a system of size L reaches the steady state at the saturation time $t_s \sim [\xi_s(L)]^{z'} \sim L^{\delta z'} \sim L^z$ and we have $z = \delta z'$. At the same token, the relationship between α and α' can be understood. The mean square fluctuation $W^2(L, t)$ of the surface height is proportional to the spacial average of $G(r, t)$. Since $G_s(r)$ in the steady state has a length scale L^δ , the square of the interface width in the steady state $W_s^2(L)$ satisfies $W_s^2(L) \sim (L^\delta)^{2\alpha'} \sim L^{2\alpha}$ and we have $\alpha = \delta\alpha'$. The extremal height suppression induces the window length scale L^δ so that α is less than α' .

There is another exponent κ which governs the behavior of $G(r, t)$ for $r^{z'} \ll t$ [9]. The scaling function $g(x)$ of Eq. (11) does not approach a constant for small values of x and, in fact, obeys the power-law scaling $x^{-\kappa}$ as shown in Fig. 2(b). The least squares fitting of $g(x)$ for small x gives $\kappa \approx 0.87$. Since $g(x) \sim x^{-\kappa}$ for small x , we expect

$$G(r, t) \sim \begin{cases} t^{2\beta} & \text{for } t \ll r^{z'} \\ r^{2\alpha' - \kappa} t^{\kappa/z'} & \text{for } r^{z'} \ll t \ll L^z \\ r^{2\alpha' - \kappa} L^{\delta\kappa} & \text{for } t \gg L^z \text{ \& } r < L^\delta \\ L^{2\alpha} & \text{for } t \gg L^z \text{ \& } r > L^\delta. \end{cases} \quad (20)$$

If one defines ‘‘local wandering exponent’’ α'_{loc} by

$$G(r, t) \sim r^{2\alpha'_{loc}} \quad (21)$$

for $r \ll \xi$ [14] then

$$\alpha'_{loc} = \alpha' - \kappa/2 \approx 0.89. \quad (22)$$

The local wandering exponent α'_{loc} describes the local width of the surface fluctuations over a size of r , where $\alpha'_{loc} \leq 1$. The boundness of α'_{loc} determining the short distance behavior of the correlation function follows from the triangle inequality argument [15].

The exponent κ can be obtained from the small x behavior of $g(x)$ in Fig. 2(b) [9]. Another way to estimate κ is to measure the mean square slope of the surface $S^2(t)$

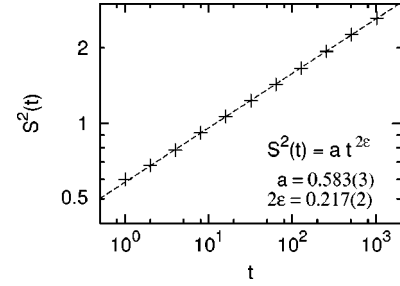


FIG. 4. The mean square slope $S^2(t)$ as a function of t for the system of $L=2048$. The least squares fit for the data with the form of $S^2(t) \sim t^{2\epsilon}$ gives $2\epsilon = 0.217 \pm 0.002$ which means $\kappa = 2\epsilon z' = 0.868 \pm 0.008$.

$= G(1, t)$ for $t < L^z$ since we have $S^2(t) \sim t^{\kappa/z'}$ for those t according to Eq. (20). Figure 4 shows the $S^2(t)$ for $t = 1, 2, 4, \dots, 1024$ with $L=2048$. All the data fit well with the form of

$$S^2(t) \sim t^{2\epsilon}, \quad (23)$$

where ϵ is a ‘‘step growth exponent’’ describing the increase of the average step height as a function of time. From the least squares fit, we get

$$2\epsilon = 0.217 \pm 0.002, \quad (24)$$

which means

$$\kappa = 0.868 \pm 0.008 \quad (25)$$

since $\kappa = 2\epsilon z'$. There is some debate about whether or not κ is an independent exponent [9,14,16,17]. In the RC model, α'_{loc} is 1 and κ is given by $2\alpha' - 2$ [9,11]. However, in our model, α'_{loc} is $\alpha' - \kappa/2$ being less than 1. We think κ is a new exponent [9,14] which cannot be derived from α' , z' , and δ .

We have shown that the measurements of α and z from the surface width is not enough to characterize a surface morphology. To classify it completely, four independent exponents α' , z' , δ , and κ are required. These four exponents can be obtained by the measurement of $G(r, t)$ as presented in Eq. (20). Still $G(r, t)$ follows the scaling behavior of Eq. (3) with

$$\xi(t) \sim \begin{cases} t^{1/z'} & \text{for } t^{1/z'} \ll L \\ L^\delta & \text{for } t^{1/z'} \gg L. \end{cases} \quad (26)$$

Exponent α' and κ are related to the asymptotic form of $g(x)$ in Eq. (3),

$$g(x) \sim \begin{cases} x^{-\kappa} & \text{for } x \ll 1 \\ x^{-2\alpha'} & \text{for } x \gg 1. \end{cases} \quad (27)$$

All other exponents α , z , β , ϵ , and α'_{loc} can be derived from the relations $\alpha = \alpha' \delta$, $z = z' \delta$, $\beta = \alpha'/z'$, $2\epsilon = \kappa/z'$, and $\alpha'_{loc} = \alpha' - \kappa/2$.

In summary, we show that the usual roughness exponent α and its dynamic exponent z from the scaling behavior of

the surface width are not enough to characterize the model. We introduce the restricted curvature model with suppression of the global extremal heights and get $\alpha \approx 0.561$ and $z \approx 1.69$ from the surface widths. However, the correlation dynamic exponent $z' \approx 4$, which describes the time dependence of the correlation length, is not the same as the usual dynamic exponent z extracted from W . We emphasize that z' is not a crossover exponent but a true exponent describing the correlation length. This unusual behavior also leads to the fact that the apparent α measured from $W(L, t)$ is different from the wandering exponent α' of the correlation. However, there is a relation among them, $\beta = \alpha/z = \alpha'/z'$. Appar-

ently different values between z and z' are due to the fact that the saturate correlation length is not the system size but is only proportional to L^δ with $\delta \approx 0.423$ which is a new exponent to describe the widow size. Just measuring the width alone is not enough to characterize the surface. Four independent exponents α' , z' , κ , and δ are required to describe the scaling behavior of the surface and they can be determined from the height correlation function.

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