Scaling function for surface width for free boundary conditions

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We study the restricted curvature model with both periodic and free boundary conditions and show that the scaling function of the surface width depends on the type of boundary conditions. When the free boundary condition is applied, the surface width shows a new dynamic scaling whose asymptotic behavior is different from the usual scaling behavior of the self-affine surfaces. We propose a generalized scaling function for the surface width for free boundary conditions and introduce a normalized surface width to clarify the origin of the superrough phenomena of the model.

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Surface roughening of crystal surfaces has been intensively studied recently using both continuum equations and discrete atomistic growth models [1–3]. Various growth models have been identified as a universality class corresponding to a particular continuum equation for the coarse grained height variables $h(x,t)$, which describes the surface as a function of the lateral surface coordinate x and time t. An interesting quantity of the dynamic growth process is the kinetically rough self-affine surface structure. The most recent work concentrates on studying the surface structure of the growth models, especially on determining the dynamic critical exponents governing the surface fluctuations. The dynamic scaling hypothesis is that the surface width W, which is the mean fluctuation of the surface height, starting from a flat substrate scales [4] as

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

in a finite system of lateral size L, where α and z are the "roughness" and "dynamic" exponents. The dynamic scaling function $g_W(u)$ usually has the following asymptotic behavior:

$$g_W(u)\sim\begin{cases}u^{\beta} & \text{for} \quad u\ll 1\\ \text{const} & \text{for} \quad u\gg 1,\end{cases} \tag{2}$$

where the growth exponent $\beta=\alpha/z$. Since $g_W(u)$ becomes constant as $u=t/L^z$ approaches infinity or t becomes much larger than L^z, we have $W\sim L^{\alpha}$ for sufficiently later times and α has been taken as the exponent representing the roughness of the stationary surface.

In general, the scaling function $g_W(u)$ as well as the exponents α and z have been taken to be independent of the type of boundary conditions. In this paper, we study the restricted curvature (RC) model [5] with free boundary conditions (FBC) and show that the scaling function of the surface width depends on the type of boundary conditions. Furthermore, we show that the scaling function of the RC model is not given in the form of Eq. (2) with FBC. The RC model is one of the simplest discrete models with super-rough surface [6,7]. Note that in the thermodynamic limit, the relative width $W(L)/L$ of the saturated surface vanishes or diverges depending on whether α is less than or greater than 1 since $W(L)/L\sim L^{\alpha-1}$. The surface of the RC model is super-rough, that is, $\alpha>1$, and the structure factor of the height follows the conventional scaling form [7]. The super-rough surfaces show "anomalous" scaling behaviors in the sense that the local roughness exponent α_{loc} [see Eq. (13)] and the global roughness exponent α are different [8]. Yet, the scaling function of the surface width has been known to be of the form of Eq. (2). Here, we show that the RC model with FBC has a different scaling behavior; the scaling function of the surface width does not follow Eq. (2). We suggest a scaling function to describe the width, and we introduce a normalized width whose scaling function is given in the form of Eq. (2) with FBC as well as in periodic boundary condition (PBC).

We study an equilibrium discrete growth model with RC constraint on the one-dimensional (1D) substrate (mainly with the FBC). Let us first explain the RC model [5] briefly for completeness. The RC model is analogous to the restricted solid-on-solid model [9], except that the restriction is on the local curvature,

$$|\nabla^2 h|=|h(x+1)+h(x-1)-2h(x)|\leqslant 2, \tag{3}$$

rather than on the height difference. The growth rule of the equilibrium RC model is to randomly select a site and to take a random action between deposition or evaporation with equal probability, provided that the new configuration does not violate the RC constraint at any site. Each update of the height results in the change of the local curvatures at three sites, the selected site and the two nearest neighbor sites. No relaxation or hopping of the deposited atom is allowed in the model, and the curvature restrictions are enforced for all the sites (except at the boundary sites for the FBC). The RC model is believed to belong to the fourth-order continuum linear equation,

$$\partial h(\mathbf{x},t)/\partial t=-\nabla^4 h(\mathbf{x},t)+\eta(\mathbf{x},t), \tag{4}$$

where $\eta(\mathbf{x},t)$ is an uncorrelated Gaussian noise. This equation can be solved exactly, giving $\alpha=\frac{3}{2}$ and $z=4$, i.e., $\beta=\frac{3}{8}$ for the 1D substrate [5,10]. The dynamics and equilibrium properties of the RC model with both PBC and FBC are studied by computer simulations. We prepare a flat surface as the initial configuration, i.e., $h(x,t)=0$ for all $x=1,\ldots,L$ at $t=0$. We then choose a site on the substrate randomly and

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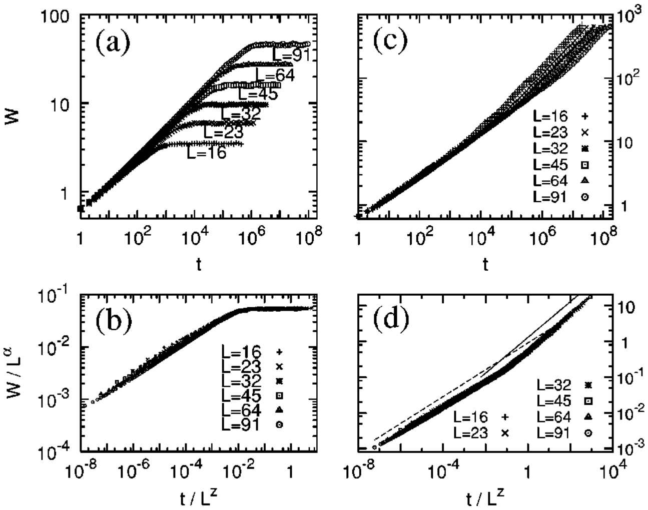

FIG. 1. (a) Surface widths $W(t,L)$ for the systems of sizes $L=16$, 23, 32, 45, 64, and 91 as a function of time t for PBC. (b) Scaling plot of W/L^{α} versus t/L^{z} with $\alpha=\frac{3}{2}$ and $z=4$ using the data shown in (a). (c) The same plots as (a) for FBC. (d) The same plots as (b) for FBC. The guide- lines are given by $y\sim x^{3/8}$ (dashed line) and $y\sim x^{1/2}$ (solid line).

try to add or subtract the height by one with the same probability $\frac{1}{2}$. The new configuration is accepted as long as it satisfies the RC conditions. One Monte Carlo step or $\Delta t=1$ is defined as L such tries (one try per site in average). We measure the surface width as

$$W(t,L)=\langle\overline{[h(t)-\bar{h}(t)]^{2}}\rangle^{1/2}, \tag{5}$$

where $\overline{A}$ and $\langle A\rangle$ represent the spatial and the sample averages of A, respectively. We first use the PBC and confirm that the surface width $W(t,L)$ shows the scaling behavior of Eqs. (1) and (2) with the roughness exponent $\alpha\approx1.5$ and the dynamic exponent $z\approx4$ [5].

Figure 1(a) shows the surface width W in PBC as a function of t, for the systems of sizes $L=16$, 23, 32, 45, 64, and 91. Initially they increase algebraically ($t\ll L^{z}$ regime) and become saturated for $t\gg L^{z}$, as expected for an usual self-affine surface. We check the validity of the scaling ansatz of Eq. (1) and (2) by plotting the scaled width W/L^{α} against the scaled time $u=t/L^{z}$. As shown in Fig. 1(b), the scaled data collapse to a single curve with $\alpha=\frac{3}{2}$ and $z=4$, supporting the scaling behavior of Eq. (1). We also see that $g_W(u)$ increases as u^{β}, for small u satisfying the asymptotic form of Eq. (2) with $\beta=\alpha/z\approx\frac{3}{8}$ in Fig. 1(b). These results seem to support the interpretation of α as an exponent to represent the roughness of the stationary surface at sufficiently later times.

Next, we apply the FBC that no restricted constraints are enforced at the boundary sites ($x=1$ and $x=L$) [11]. Figure 1(c) shows W versus t plots for the FBC case. The width increases as $t^{3/8}$ at the beginning, being the same as the PBC case, but keeps on increasing as $t^{\beta'}$ (with another exponent β') at a later time $t\gg L^{z}$, where W is never saturated to a constant, in contrast to the case of the PBC. We propose a scaling formula for the FBC,

$$W(t,L)\sim L^{\alpha}g'_W(t/L^{z}), \tag{6}$$

with a generalized dynamic scaling function $g'_W(u)$ which has the following asymptotic behavior:

$$g'_W(u)\sim\begin{cases}u^{\beta} & \text{for} \quad u\ll1,\\ u^{\beta'} & \text{for} \quad u\gg1,\end{cases} \tag{7}$$

so that the asymptotic form of the surface width is given by

$$W(t,L)\sim\begin{cases}t^{\beta} & \text{for} \quad t\ll L^{z},\\ t^{\beta'}/L^{z(\beta'-\beta)} & \text{for} \quad t\gg L^{z}.\end{cases} \tag{8}$$

In most of the growth models, $\beta'=0$, and the scaling function g'_W of Eq. (7) reduces to the usual form of Eq. (2). However, we find that $\beta'\approx\frac{1}{2}$ for the RC model with the FBC. When the scaled width W/L^{α} is plotted against the scaled time $u=t/L^{z}$ with $\alpha=\frac{3}{2}$ and $z=4$, the surface widths collapse to a single curve following the scaling behavior of Eq. (6) as shown in Fig. 1(d). The scaling function g'_W increases as $u^{3/8}$ for small u, and $u^{1/2}$ for large u. [The slopes of the dashed and solid lines in Fig. 1(d) are $\frac{3}{8}$ and $\frac{1}{2}$, respectively.] Therefore, the surface width $W(t,L)$ has the following anomaly:

$$W(t)\sim\begin{cases}t^{3/8} & \text{for} \quad t\ll L^{z},\\ t^{1/2}/L^{1/2} & \text{for} \quad t\gg L^{z},\end{cases} \tag{9}$$

in the FBC. It is interesting that the surface width is not saturated even for $t\gg L^{z}$. This is due to the boundary condition—in FBC, the overall tilt of the surface is allowed, whereas it is not allowed, in PBC. For $t\gg L^{z}$, W behaves like a random deposition problem so that W grows as $t^{1/2}$. Even though the surface width is not saturated for $t\gg L^{z}$, the roughness exponent α can be calculated through the relation $\alpha=z\beta$. This α is independent of the type of boundary conditions.

We emphasize that the type of boundary conditions usually do not affect the form of scaling functions as well as the dynamic exponents. To confirm this, we measure the surface width of the Family model [4] with PBC. The growth algorithm is to select one substrate site randomly at each time step and then drop one particle to the selected site. The dropped particle is allowed to diffuse to one of the nearest neighbor sites that have lower height as compared to the height of the selected site. It is known that the model has $\alpha=\frac{1}{2}$ and $z=2$ with PBC. In the model with FBC, we find $\beta'=0$. The saturated surface width in FBC is a little bit larger than that in PBC but W follows the ordinary scaling [Eq. (2)] with the same values of the exponents in PBC. Even in FBC, it seems that the overall tilt of the surface is not allowed according to the growth rules of the model. It is usual that the scaling functional form does not depend on the type of boundary conditions. However, we show that the width of the RC model follows a scaling behavior in FBC.

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 [9],

$$G(r,t,L)=\langle[h(x,t)-h(x+r,t)]^{2}\rangle. \tag{10}$$

The scaling behavior of the correlation function is given by

$$G(r,t,L) \sim r^{2\alpha} g_G(r/\xi(t,L)), \tag{11}$$

where ξ is the correlation length. The exponent z governs the dynamics of the correlation length along the surface, which grows as $t^{1/z}$ at the beginning and eventually becomes saturated at the system size L.

It has been known that the scaling function $g_G(u)$ for the RC model does not approach a constant as u goes to zero but shows a power-law scaling $u^{-\kappa}$ [6,12] with a nonzero κ, which governs the behavior of $G(r,t,L)$ for $r^z \ll t$. There is some debate about whether or not κ is an independent exponent [6,7,12–14]. Since $g_G(u) \sim u^{-\kappa}$ for small u, we expect [6,12]

$$G(r,t,L) \sim \begin{cases} t^{2\beta} & \text{for} \quad t \ll r^z, \\ r^{2\alpha-\kappa} t^{\kappa/z} & \text{for} \quad r^z \ll t \ll L^z, \\ r^{2\alpha-\kappa} L^{\kappa} & \text{for} \quad t \gg L^z, \end{cases} \tag{12}$$

in PBC. If one defines "local wandering exponent" α_{loc} by

$$G(r,t,L) \sim r^{2\alpha_{loc}} \tag{13}$$

for $r \ll \xi$ [7,12], then α_{loc} is given by

$$\alpha_{loc} = \alpha - \kappa/2, \tag{14}$$

from Eq. (12). The local wandering exponent α_{loc} describes the local width of the surface fluctuations over a size of r, where $\alpha_{loc} \leqslant 1$. The boundness of α_{loc} determining the short distance behavior of the correlation function follows from the triangle inequality argument [15]. It is known that $\alpha_{loc} = 1$ and $\kappa = 1$ in the RC model [6].

Here, we concentrate on $G(r,t,L)$, with $r=1$, which represents the height difference between the neighboring columns [12]. The local slope $S(t,L)$, defined as the root mean square of the height difference between the neighboring columns,

$$S(t,L) = \sqrt{G(1,t)}, \tag{15}$$

is expected to have the scaling form of

$$S(t,L) \sim L^{\alpha_s} g_S(t/L^{z_s}), \tag{16}$$

where α_s and z_s are the "roughness" and "dynamic" exponents for the slope. For the PBC case, we see that the dynamic scaling function $g_S(u)$ for the slope has the following asymptotic behavior:

$$g_S(u) \sim \begin{cases} u^{\alpha_s/z_s} & \text{for} \quad u \ll 1, \\ \text{const} & \text{for} \quad u \gg 1, \end{cases} \tag{17}$$

with $\alpha_s = \kappa/2$ and $z_s = z$ from Eq. (12). Note that we have only one dynamic exponent here, $z = z_s = 4$.

Figure 2(a) shows the local slope versus t graph for the system of the sizes $L=16$, 23, 32, 45, 64, and 91 with PBC. They increase algebraically initially ($t \ll L^z$ regime) and become saturated for $t \gg L^z$. The rescaled slopes S/L^{α_s} collapse to a single curve when they are plotted against the rescaled time $u = t/L^{z_s}$ with $\alpha_s = \frac{1}{2}$ and $z_s = 4$, as shown in Fig. 2(b). The rescaled graph increases as u^{β_s} initially, and then saturates for $u \gg 1$, where $\beta_s = \alpha_s/z_s = \frac{1}{8}$. Therefore, the asymptotic behavior of $S(t,L)$ is given by

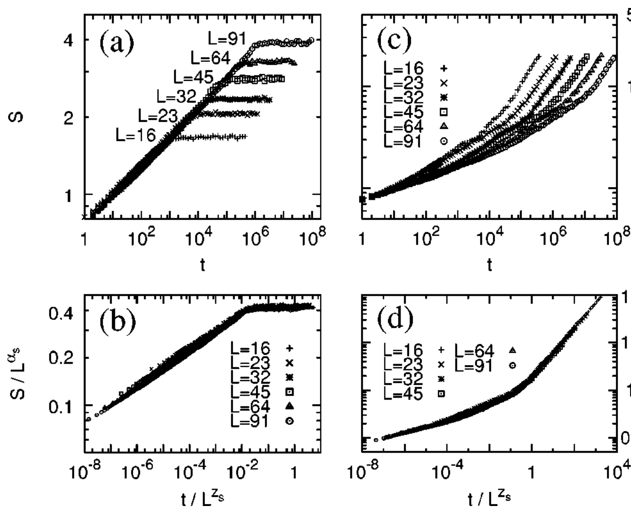

FIG. 2. (a) The root mean square slopes $S(t,L)$ for the systems of sizes $L=16$, 23, 32, 45, 64, and 91 plotted against time t for PBC. (b) Scaling plot of S/L^{α_s} versus t/L^{z_s} with $\alpha_s = 1/2$ and $z_s = 4$ from the data shown in (a). (c) The same plots as (a) for FBC. (d) The same plots as (b) for FBC.

$$S(t,L) \sim \begin{cases} t^{1/8} & \text{for} \quad t \ll L^4, \\ L^{1/2} & \text{for} \quad t \gg L^4, \end{cases} \tag{18}$$

for the PBC case. Note that the local slope S saturates to $L^{1/2}$ for $t \gg L^4$. Since there is a restriction only on the curvature, the height difference between the nearest neighbors can be arbitrarily large. For $1 \ll t \ll L^z$, the slope $S(t,L)$ increases as $t^{1/8}$ and eventually saturates, being proportional to $L^{1/2}$ when the parallel correlation $t^{1/z}$ is of the order of the lateral system size L. The reason that $S(t)$ saturates for $t > L^z$ is because the boundary condition effectively sets the upper bound of $S(t)$ as $\sim \sqrt{L}$.

We also apply the FBC and measure the nearest neighbor height difference. Figure 2(c) shows $S(t,L)$ versus t graph for the FBC case. The local slope S increases as $t^{1/8}$ initially, as in the PBC case. However, it keeps on increasing for $t > L^z$, unlike in the PBC case. Still, $S(t,L)$ shows a scaling behavior as shown in Fig. 2(d). When the scaled slope S/L^{α_s} is plotted against the scaled time t/L^z with $\alpha_s = \frac{1}{2}$ and $z = 4$, the data collapse to a single curve, indicating that S also follows the scaling ansatz,

$$S(t,L) \sim L^{\alpha_s} g'_S(t/L^z), \tag{19}$$

where the scaling function $g'_S(u)$ is proportional to u^{β_s} for small u, and $u^{\beta'_s}$ for large u with $\beta_s = \frac{1}{8}$ and $\beta'_s \approx \frac{1}{2}$. Therefore, the local slope in FBC shows

$$S(t,L) \sim \begin{cases} t^{1/8} & \text{for} \quad t \ll L^4 \\ t^{1/2}/L^{3/2} & \text{for} \quad t \gg L^4, \end{cases} \tag{20}$$

and increases as $\sim t^{1/2}$ at later times. The change of the growth exponent from $\beta_s = \frac{1}{8}$ to $\beta'_s = \frac{1}{2}$ occurs when the correlation length becomes the same as the system size.

Since both the scaling forms of $W(t,L)$ and $S(t,L)$ depend on the types of boundary conditions, we can consider a normalized surface width

$$W_N(t,L) = W(t,L)/S(t,L), \tag{21}$$

which represents the surface width in units of the nearest neighbor height difference [12]. From the above scaling formula [Eqs. (1), (6), (16), and (19)], we expect

$$W_N(t,L) \sim L^{\alpha-\alpha_s} g_N(t/L^z) \sim \begin{cases} t^{\beta_N} & \text{for} \quad t \ll L^z, \\ L^{\alpha_{loc}} & \text{for} \quad t \gg L^z, \end{cases} \tag{22}$$

where $\beta_N = \beta - \alpha_s/z = \frac{1}{4}$ and $\alpha_{loc} = \alpha - \alpha_s = 1$ for the RC model. The local wandering exponent can be obtained from $W_N(L)$ in $t \gg L^z$. We expect that the scaling formula of Eq. (22) is valid for both PBC and FBC.

In PBC, the normalized width $W_N(L)$ and the slope $S(L)$ become $L^{\alpha_{loc}}$ and L^{α_s}; respectively, as t goes to infinity, so $W(L) \sim W_N(L) S(L) \sim L^{\alpha_{loc}+\alpha_s} \sim L^{\alpha}$, with $\alpha = \alpha_{loc} + \alpha_s$. The reason that $\alpha > 1$ is because the saturated slope $S(\infty, L)$ depends on L in PBC. In FBC, the normalized width $W_N(L)$ saturates to $L^{\alpha_{loc}}$, but the slope $S(t,L)$ increases as $t^{1/2}$ as t goes to infinity, so the width $W(t,L)$ diverges as $t^{1/2}$. Therefore, the average slope can be a natural unit for measuring the height in the RC model [12] so that the scaling functions of the surface width in terms of the average slope are insensitive to the boundary conditions.

We measure the surface width in the RC model for free boundary conditions and find a different scaling behavior of W. The asymptotic behaviors of W and S in a discrete model which has nonzero α_s can depend on the type of the boundary conditions. In FBC, the width grows as t^{β} at the beginning and keeps on increasing as $t^{\beta'}$ with different power law at later times. The surface width is not saturated but the roughness exponent α can be defined by the relation $\alpha = z\beta$. W shows a different scaling behavior compared to the Family-Vicsek–type scaling [4]. However, if we consider the normalized surface width, it returns to the ordinary Family-Vicsek–type scaling. These scaling behaviors of W and S in FBC have not been shown before. In other models, such as the Family model [4] or restricted solid-on-solid growth model [9], β' is always zero, so that the surface width is saturated at later times, being independent of the type of boundary conditions. In the RC model, the nonzero α_s is because of there being no restriction on the nearest neighbor height difference. Since the saturated width $W(L)$ is proportional to $S(L)L^{\alpha_{loc}}$, where S is the root mean square of the nearest neighbor height difference, the roughness exponent α is the sum of α_{loc} and α_s. This is the reason why α can be different from α_{loc}.

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