

Kinetic roughening on rough substrates

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We study the kinetic roughening described by a linear diffusion equation on an initially rough substrate. We show analytically that it is not possible to write a general scaling relation valid for rough substrates. However, for a particular substrate generated by the same linear growth process, we can write a scaling relation similar to the relation valid for flat substrates, with the same growth and roughness exponents. Numerical simulations in a solid-on-solid model with surface relaxation, for $d=1$, supports the scaling relation and the exponents. [S1063-651X(97)09710-9]

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Kinetic roughening in nonequilibrium surface growth is a problem that has been extensively studied in the past decade [1–6]. Some experimental examples are the fluid-fluid interface in porous medium [7,8], paper wetting [9], propagation of flame fronts [10,11], fractures [12], molecular-beam epitaxy [4,13], and growth of bacterial cell colonies [14]. The standard theoretical methods for treating these problems are continuum equations [15,16], scaling concepts [17], and a great variety of discrete models [17,18,25,19,20].

A simplified yet nontrivial equation to describe kinetic roughening has been introduced by Kardar, Parisi, and Zhang [16]. The height $h(\mathbf{x},t)$ of the profile in position \mathbf{x} at time t evolves as

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu \nabla^2 h(\mathbf{x},t) + \frac{\lambda}{2} [\nabla h(\mathbf{x},t)]^2 + \eta(\mathbf{x},t), \quad (1)$$

where the first term is related to the surface relaxation, the second simulates the lateral growth, and $\eta(\mathbf{x},t)$ is a white noise with zero mean and covariance given by

$$\langle \eta(\mathbf{x},t) \eta(\mathbf{x}',t') \rangle = 2D \delta^d(\mathbf{x} - \mathbf{x}') \delta(t - t'), \quad (2)$$

where the angular brackets denote an average over noise histories and d is the dimension of the substrate.

In 1985 Vicsek and Family [17] predicted spatial and temporal scaling properties for the interface of crystal growth. For a discrete interface of L^d sites, where the site i has a height h_i , we can define the interface width, also called roughness, as

$$w^2(t,L) = \frac{1}{L^d} \sum_{i=1}^{L^d} (h_i - \bar{h})^2, \quad (3)$$

where $\bar{h} = (1/L^d) \sum h_i$ is the mean height. For a particle deposition process in an initially flat substrate this roughness behaves as [17]

$$w(t,L) \sim L^\alpha f\left(\frac{t}{L^z}\right), \quad (4)$$

where α is the roughness exponent and z is the dynamical exponent. When $0 \ll t \ll L^z$, the function $f(t/L^z)$ behaves as

$f(t/L^z) \sim (t/L^z)^\beta$, where $\beta = \alpha/z$ is the growth exponent. Then the roughness has the dynamical behavior $w(t,L) \sim t^\beta$ for short times. For $t \gg L^z$, the function $f(t/L^z) = \text{const}$ and $w(\infty,L) \sim L^\alpha$. In this limit, the interface has a self-affine character.

In a growth process where the lateral growth is important, the λ term in Eq. (1) dominates. In that case, the relation $\alpha + z = 2$ is valid for all dimensions and the exact solution is known only for 1+1 dimensions, with $\alpha = 1/2$ and $\beta = 1/3$. On the other hand, if the ν term dominates, Eq. (1) reduces to a linear equation with exact solution: $z = 2$, $\alpha = (2 - d)/2$, and $\beta = (2 - d)/4$. All of these results are valid for a flat substrate. However, as pointed out by Meakin [3], growth from an initially rough substrate is probably more common in nature. The growth in a disordered substrate was studied theoretically by Tsai and Shapir [21], while the formation of a facet on an initially rough surface was investigated by Krug and Spohn [22].

In this Brief Report, we report analytic results of a linear equation in a rough substrate, with roughness $w_0(L)$, and we show that it is not possible to establish a general scaling relation. However, for a particular substrate, we show that $w^2(t,L) - w_0^2(L)$ obeys a scaling relation identical to Eq. (4), which is valid for flat substrates. We perform numerical simulations in a one-dimensional model of the same universality class, the solid-on-solid (SOS) model with surface relaxation [15,18]. The results obtained validate the theoretical scaling relation.

We consider Eq. (1) with $\lambda = 0$, that is, the linear equation

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu \nabla^2 h(\mathbf{x},t) + \eta(\mathbf{x},t). \quad (5)$$

This equation has an exact solution and the roughness $w(t,L)$ can be expressed as [6,23]

$$w^2(t,L) = \int \frac{d\mathbf{q}}{(2\pi)^d} \int \frac{d\mathbf{q}'}{(2\pi)^d} C_{\mathbf{q},\mathbf{q}'}(t), \quad (6)$$

where the correlation $C_{\mathbf{q},\mathbf{q}'}(t) \equiv \langle h(\mathbf{q},t) h(\mathbf{q}',t) \rangle$ is given by

$$C_{q,q'}(t) = \left[e^{-2\nu q^2 \Delta t} C_{q,q'}(t_0) + \frac{(2\pi)^d D}{2\nu q^2} \right] \times (1 - e^{-2\nu \Delta t q^2}) \delta^d(\mathbf{q} + \mathbf{q}'), \quad (7)$$

with $\Delta t = t - t_0$. For a flat substrate $C_{q,q'}(t_0) = 0$ and the roughness is given by

$$w^2(t, L) = \frac{D}{2^d \nu \pi^{d/2} \Gamma\left(\frac{d}{2}\right)} \int_{\frac{2\pi}{L}}^{\infty} \frac{dq}{q^{3-d}} (1 - e^{-2\nu t q^2}). \quad (8)$$

For $d=1$ this expression can be written in the scaling form

$$w^2(t, L) = \frac{DL}{\nu} f\left(\frac{\nu t}{L^2}\right), \quad (9)$$

where, for small $x \equiv \nu t/L^2$, we have $f(x) \sim x^{1/2}$ ($w \sim t^{1/4}$) and $f(x)$ tends to a constant for large x ($w \sim L^{1/2}$). For $d=2$, the roughness has the logarithmic behaviors [23] $w(t, L) \sim \ln t$ for small t and $w(t, L) \sim \ln L$ for long times.

For a rough substrate we have $C_{q,q'}(t_0) \neq 0$ and it is impossible to obtain a general scaling relation such as Eq. (9) for any initial substrate. For example, in an uncorrelated growth process [$\nu=0$ in Eq. (5)] the correlation is given by

$$C_{q,q'}(t_0) = (2\pi)^d D t_0 \quad (10)$$

and Eq. (6) cannot be expressed as a scaling relation.

Nevertheless, if the correlation function has the form $C_{q,q'}(t_0) \sim q^{-2}$, then it is possible to write down a scaling relation similar to Eq. (9). A substrate with such a correlation function can be generated by the same growth process (5) on a flat substrate. In that case, we use a coefficient ν_0 until the time is long enough ($t \gg L^2$). Under these conditions, Eq. (7) reads

$$C_{q,q'}(t_0) = \frac{(2\pi)^d D}{2\nu_0 q^2} \delta^d(\mathbf{q} + \mathbf{q}'). \quad (11)$$

By substituting this equation into Eq. (6) we obtain

$$w_0^2(L) = \frac{D}{2^d \nu_0 \pi^{d/2} \Gamma\left(\frac{d}{2}\right)} \int_{\frac{2\pi}{L}}^{\infty} \frac{dq}{q^{3-d}}. \quad (12)$$

Therefore, once the process starts on a substrate generated under those conditions, we find that the fluctuation in roughness

$$\delta w^2 = |w^2(t, L) - w_0^2(L)| \quad (13)$$

can be expressed as

$$\delta w^2 = \frac{D}{2^d \pi^{d/2} \Gamma\left(\frac{d}{2}\right)} \left| \frac{1}{\nu} - \frac{1}{\nu_0} \right| \int_{\frac{2\pi}{L}}^{\infty} \frac{dq}{q^{3-d}} (1 - e^{-2\nu t q^2}). \quad (14)$$

This relation is identical to Eq. (8) for flat substrates with effective coefficient ν_{eff} defined as

$$\frac{1}{\nu_{eff}} = \left| \frac{1}{\nu} - \frac{1}{\nu_0} \right|. \quad (15)$$

Hence the same scaling relation is obeyed. Then, for $d=1$ the scaling relation valid for this kind of substrate is

$$\delta w^2 = \frac{DL}{\nu_{eff}} f\left(\frac{\nu t}{L^2}\right). \quad (16)$$

A similar scaling relation was obtained by Kertész and Wolf for the Eden model [24]. However, the Kertész-Wolf relation depends of the intrinsic roughness of the model that is L independent, while in the present work the initial roughness $w_0(L)$ grows with L .

In order to understand the above results we perform a simulation with a model of the same universality class, the so-called SOS model with surface relaxation, in $d=1$. That model was introduced by Edwards and Wilkinson [15], who determined the exponents analitically. Family [18] obtained numerical results that support the scaling relation (4) with the same exponents. A site i is select at random and its height h_i grows one unit, that is, $h_i \rightarrow h_i + 1$, provided that the restriction on neighboring heights $h_i - h_{i\pm 1} < m$ is obeyed at all stages. In this constraint, m is a parameter related to the coefficient ν . In case the constraint is violated, the lowest neighboring site is visited until a local minimum is reached. A substrate is generated by this process by using a value m_0 until a steady state ($t \gg L^2$) is attained. On that

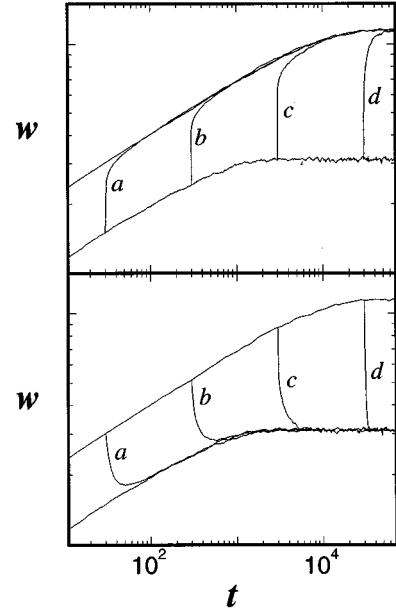


FIG. 1. The log-log plots of the roughness $w(t, L)$ as a function of t for $L=200$. In both parts, we show the growth process in a flat substrate for $m=1$ (lower curve) and for $m=5$ (upper curve). On the top roughening processes from $m=1$ to $m=5$ and on the bottom smoothing processes from $m=5$ to $m=1$ are described. The segments a , b , c , and d show the behavior when we change the parameter m at times $t=30$, 300 , 3000 , and $30\,000$, respectively.

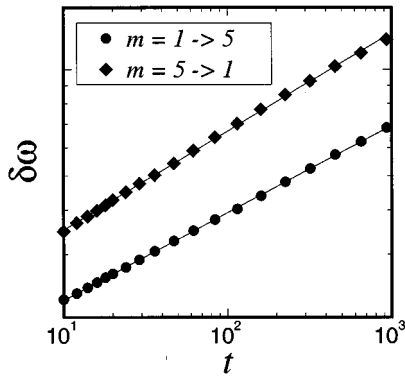


FIG. 2. The log-log plots of the fluctuation in roughness δw as a function of t in two process: (a) roughening (lower curve) (in an $L=800$ less rough substrate, generated with $m=1$, grows a structure with $m=5$) and (b) smoothing (upper curve) (in an $L=800$ very rough substrate, generated with $m=5$, grows an interface with $m=1$).

substrate another growth process will begin with another maximum height difference $m \neq m_0$. The change in the parameter m corresponds to a change in the coefficient ν . For instance, a low value of m means a less rough substrate, that is, a higher value of the coefficient ν .

Figure 1 shows log-log plots of the roughness $w(t, L)$ vs time t for $L=200$. The lower (upper) curves are for $m=1$ ($m=5$). The segments *a*, *b*, *c*, and *d* on the top describe the roughening from $m=1$ to $m=5$ at different times. The segments on the bottom describe the smoothing processes $m=5$ to $m=1$. We note that there exists a tendency of the roughness to go quickly to the corresponding curve of the new value of m . Even for the smoothing process the segment *a* shows a strong decreasing of the roughness and then it returns to the ascending curve.

Figure 2 shows the absolute value of the fluctuations of roughness δw vs time t for two growth process: (a) roughening, a process with $m=5$ on a less rough substrate generated with $m_0=1$, and (b) smoothing, a process with $m=1$ on a very rough substrate generated with $m_0=5$. For each one, we have generated 30 substrates and 30 growth processes for each substrate. Hence we used effectively 900 samples. The results shown are for $L=800$. The curves are in

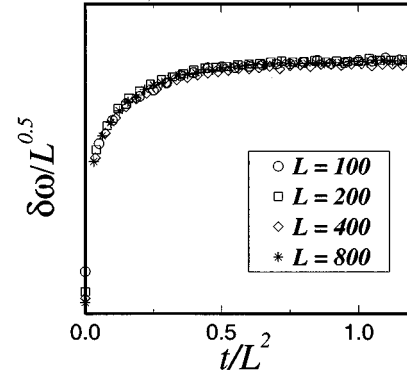


FIG. 3. Plots of $\delta w/L^{1/2}$ vs t/L^2 for various values of L showing the validation of the scaling relation (16).

good agreement with $2\beta=0.48 \pm 0.02$ for roughening and $2\beta=0.51 \pm 0.03$ for smoothing, which indicates $\beta \approx 1/4$, as expected. The validation of the scaling relation (16) can be inferred from Fig. 3: Plots of $\delta w/L^{1/2}$ vs t/L^2 , for several values of L , collapse on the same curve, which indicates that $f(x)$ is L independent.

In conclusion, we analyze the kinetic roughening on an initially rough substrate. Through a solution of a linear diffusion equation we show that it is impossible to obtain a general scaling relation as such Eq. (9), which is valid for flat substrates. Nevertheless, for a particular substrate generated by the same linear process but with a different coefficient ν , we can write down a similar scaling relation (16) which is a generalization of Eq. (9). It is possible to study analytically other models that are related to a linear equation of higher order [19,20] and to obtain similar results. Numerical simulations in a SOS model with surface relaxation, where a difference m of height between neighbors is allowed, indicate the correctness of this scaling relation. We also perform numerical simulations in a SOS model with refuse [25] to see the results of a nonlinear model on a rough substrate.

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