Conserved growth model with a restricted solid-on-solid condition in higher dimensions

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A conserved growth model with a constraint on neighboring interface heights in substrate dimensions $d_s = 2,3,4,5$ is investigated. A randomly dropped particle is allowed to hop to the nearest site satisfying the restricted solid-on-solid condition. The scaling properties of the surface in $d_s = 2, 3$, and 4 are consistent with those of the continuum equation $\partial h/\partial t = -\nu \nabla^4 h + \lambda \nabla^2 (\nabla h)^2 + \eta$. The upper critical dimension of the model is also discussed. [S1063-651X(97)10110-6]

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Recently there has been great interest in the dynamic properties of the interfaces of various growth models [1]. An interesting physical property of the dynamic growth process is the kinetically rough self-affine surface structure. Most of the recent work concentrated on studying the surface structure of the growth models, especially on determining the dynamical critical exponents governing the surface fluctuations [1]. The dynamic scaling hypothesis is that in a finite system of lateral size L, the standard deviation or the root mean square fluctuation W of the surface height starting from a flat substrate scales as [2]

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

where the scaling function f(x) is x^{β} (with $\beta = \alpha/z$) for $x \ll 1$ and is constant for $x \gg 1$.

Among the growth models the restricted solid-on-solid (RSOS) model [3,4], in which the differences between the neighboring heights of the local columns are usually restricted to zero or unity in magnitude, has been intensively studied. Even with this restriction, the equilibrium RSOS model still exhibits a roughening transition [3] and the non-equilibrium growth model [4] follows the Kardar-Parisi-Zhang (KPZ) equation [5–7] rather well.

Recently there have been considerable efforts in conserved growth models, in which the number of particles are conserved after being deposited, because of the possible relevance to the real molecular beam epitaxial (MBE) growth [8–16]. We have also studied a conserved growth model with the RSOS condition [17,18]. The growth algorithm of the ''conserved RSOS (CRSOS) model'' is very similar to the simple RSOS model [4] except for a relaxation process. The growth rule is following: (I) A site \vec{x} is selected randomly on a d_s -dimensional substrate. (II) If the restricted solid-on-solid condition on the neighboring heights $|\delta h| = 0, 1, \ldots, N$ is obeyed after a particle is deposited at \vec{x} , where N is a preassigned restriction parameter, then a growth is permitted by increasing the height $h(\vec{x}) \rightarrow h(\vec{x}) + 1$. (III) If the RSOS condition is not obeyed at the position \vec{x} , the dropped particle is allowed to hop to the nearest site where the RSOS condition is satisfied. If there is more than one neighboring site at the same distance from \vec{x} that satisfies the RSOS condition, one of them is chosen randomly.

Extensive studies on various physical properties, such as the surface width, the distribution of hopping distances, and the tilt-dependent surface current of the CRSOS model in the substrate dimension $d_s = 1$ [18], have shown that the CRSOS model follows the conserved KPZ equation [8,11,16]

$$\frac{\partial h(x,t)}{\partial t} = -\nu_4 \nabla^4 h(x,t) + \lambda \nabla^2 (\nabla h)^2 + \eta(x,t), \quad (2)$$

where

$$\langle \eta(x,t) \eta(x',t') \rangle = 2D \,\delta(x-x') \,\delta(t-t').$$
 (3)

The one-loop renormalization group (RG) calculations with conserved [16] or nonconserved noises [8] have shown that the value of the roughness exponent α and the value of the dynamic exponent z in Eq. (2) satisfy the scaling law

$$\alpha + z = 4, \tag{4}$$

and have claimed that the λ of Eq. (2) is not renormalized under the RG transformation so that the scaling law (4) is exact [8,16]. There is the other scaling relation derived from the surface current conservation [9,16,8]

$$z - 2\alpha - d_s = 0, \tag{5}$$

where d_s is the substrate dimensions. From both Eq. (4) and Eq. (5) one can get the supposedly exact values of the exponents:

$$\alpha_e = (4 - d_s)/3, \quad z_e = (8 + d_s)/3,$$

$$\beta_e = \alpha_e/z_e = (4 - d_s)/(8 + d_s). \tag{6}$$

However, recently Janssen [19] has claimed that the scaling relation (4) was derived from an ill-defined transformation [8,16] and the relation should be modified as

$$\alpha + z = 4 - 3\,\delta. \tag{7}$$

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The two-loop RG calculation [19] has shown that δ is very small ($\delta \le 0.03$) for $d_s = 1,2,3$ and $\delta = 0$ for the upper critical substrate dimension $d_s^c = 4$ where $\alpha = 0$ and $\beta = 0$. If there exists such a correction, then the true values of the exponents α, z, β for Eq. (2) are expected to be slightly smaller than the corresponding values in Eq. (6).

In this paper we present the simulation results for the CRSOS model on substrate dimensions $d_s=2$, 3, 4, and 5. The motivation of our study is to check whether the CRSOS model on higher-dimensional substrates also follows Eq. (2) or not. The RG calculations [8,19] for Eq. (2) have predicted that the upper critical dimension d_s^c is four. We have measured the surface roughness W(t) of the CRSOS model in higher dimensions and found that $W \sim \ln t$ in $d_s=4$. From the theoretical point of view it should be very interesting to find whether the scaling relation (4) is exact or not, even though the correction term δ of Eq. (7) is probably quite small. So the other motivation of our study is to compare Janssen's correction [Eq. (7)] with the value of exponents in the CRSOS model.

There are several ways to simulate the CRSOS model on the d_s -dimensional lattice due to the growth rule (III). Consider the CRSOS model on a two-dimensional square lattice. If a site of coordinate (x, y) is selected and the site does not satisfy the RSOS condition, then we should seek the nearest site that satisfies the RSOS condition for the growth. When searching for the nearest sites, we should choose one distance measure among the several possible distance measures in the square lattice. One possible measure is the real distance (RD) measure. If one uses the RD measure, the distance between (x,y) and (a,b) is $\sqrt{(x-a)^2+(y-b)^2}$. The other possible measure is the chemical (lattice-bond) distance (CD) measure. If one uses the CD measure, the distance between (x, y) and (a, b) is |x-a| + |y-b|. In the CD measure, all eight next nearest neighbors of (x, y), i.e., the sites at $(x \pm 1, y \pm 1)$, $(x \pm 2, y)$, and $(x, y \pm 2)$, have the same distance away from (x, y), but in the RD measure those at $(x \pm 1, y \pm 1)$ are nearer to (x, y) than those at $(x \pm 2, y)$ and $(x, y \pm 2).$

Let us first discuss the results of the simulations on a square lattice $(d_s=2)$. Our simulations have been done mainly for the restriction parameter N=1. As explained in the previous paragraph, we can think of two versions of the CRSOS model, one based on the CD measure and the other on the RD measure. The simulations are performed from a flat square lattice with the periodic boundary condition. To determine the growth exponent β , we have measured the root mean square fluctuations W(L,t) of $h(\vec{x},t)$ as a function of the ordinary Monte Carlo time t for a substrate size $L \times L = 256 \times 256$, averaging over 100 independent runs. The data for CRSOS models based on both the CD measure and the RD measure are shown in Fig. 1. Using the relation $W \sim t^{\beta}$ for $t \ll L^{z}$ [1] and the data for lnt>5 in Fig. 1, we have obtained

$$\beta = 0.19 \pm 0.01$$
 (CD), $\beta = 0.18 \pm 0.01$ (RD)
for $d_s = 2$.

As one can see from Fig. 1, the data for CD measure are slightly smaller than those for RD measures, but the gap

(8)



FIG. 1. Surface width W of the CRSOS model as a function of time in log-log plot on a square lattice $(L \times L = 256 \times 256)$. CD means the data for the model based on a chemical distance measure and RD means the data for the model based on a real distance measure. The solid lines are the lines corresponding to $\beta = 0.18$ and $\beta = 0.19$, respectively.

between the data decreases as a function of time. As one expected, the modification of the distance measures does not change the universality of the model. The values of β for both measures approach around 0.19 for $\ln t > 8$. The values of β are close to, but smaller than, $\beta_e = 1/5$ in $d_s = 2$ [see Eq. (6)].

To get an estimation of δ , the simulations for the model based on the CD measure have been done on a larger square lattice substrate with the size $L \times L = 800 \times 800$ and the results are shown as the plot of $\ln W/t^{0.2}$ againtst $\ln t$ in Fig. 2. Then we have measured the successive slope $(-\gamma)$ of the curve as a function of 1/t and extrapolated the slope $(-\gamma)$ to $t = \infty$, where $\gamma = 0.2 - \beta$ is around 0.013. So we have obtained $\delta \approx 0.065$. In a similar way, from the lnW versus lnt plot, we have also measured the successive slope of β as a function of 1/t. The extrapolated value of β is around 0.19 with $\delta \approx 0.05$. We have found that there is a consistent trend of nonzero δ . The estimated values are somewhat larger than Janssen's value of 0.014 in $d_s = 2$ [19]. One of the possible explanations for the larger value of δ is due to the systematic small size effects. More large simulations in other dimensions are required.

For the exponent α , we have used the relation $W(L,t) \sim L^{\alpha}$ in the steady-state regime $t \gg L^{z}$ [1]. We have used the system sizes L=16,24,32,47,64 for the measurement of $W(L,t=\infty)$ in the steady-state regime. From the data shown in Fig. 3, we have obtained

$$\alpha = 0.63 \pm 0.02$$
 (CD), $\alpha = 0.60 \pm 0.02$ (RD) $(d_s = 2)$.
(9)

As shown in Fig. 3, $W(\infty)$'s with CD measure are slightly smaller than those with RD measure for the smaller system sizes. The gap between them decreases as *L* increases. So we



FIG. 2. Plot of $\ln(W/t^{0.2})$ against $\ln t$ for $d_s = 2$. The data for W in this figure are taken for the model based on the CD measure on a square lattice with the size $L \times L = 800 \times 800$.

expect that α 's for both measures also approach commonly around 0.62 for larger *L*. This result for α is also close to, but smaller than, $\alpha_e = 2/3$ for $d_s = 2$ [see Eq. (6)]. Since the estimated error is somewhat large, we could not exclude the values in Eq. (6) through the numerical simulation only. From Eqs. (8) and (9), we can get $z \approx 0.63/0.19 \approx 3.32$ and $\alpha + z \approx 3.95$ for the CD measure and $z \approx 0.6/0.18 \approx 3.33$ and $\alpha + z \approx 3.93$ for the RD measure. Even though the values of α are smaller than 2/3, the values of $\alpha + z$ are very close to 4. If there are some corrections for the scaling relation $\alpha + z = 4$, then they are probably very small.

To get an estimation of δ from $W(\infty)$, we have plotted $\ln W/L^{2/3}$ against L as shown in Fig. 4. The slope of this plot



FIG. 3. W in a steady-state regime on a square lattice as a function of the substrate size L in a log-log plot.



FIG. 4. Plot of $\ln W/L^{2/3}$ against $\ln L$ for the steady-state regime. The negative slope of the guide line is corresponding to $\delta = 0.05$.

should be $(-\delta)$. The slope of the fitted line in Fig. 4 is around -0.05. Thus the estimated δ from $W(\infty)$ is close to the value from the analysis of time-dependent width W. It is also somewhat larger than Janssen's value of 0.014 in $d_s = 2$.

We have also investigated the correlation function $G(r,t) = \langle [h(\vec{x}+\vec{r},t)-h(\vec{x},t)]^2 \rangle$ of the CRSOS model. As shown in Fig. 5, the correlation function of the model based on the CD measure satisfies the scaling relation $G(r,t) = r^{2\alpha} f(r/t^{1/z})$ well if one use the values of exponents α and $z = \alpha/\beta$ in Eqs. (8) and (9). We have also confirmed that the correlation function for the RD measure also satisfies the corresponding scaling law well.



FIG. 5. The data collapse of the scaled height-height correlation functions G(r,t) on a square lattice for $t=10,20,\ldots,130$ with $\alpha=0.63$ and z=3.32. The data are for the CRSOS model based on the CD measure.



FIG. 6. Surface width W of the CRSOS model as a function of time in log-log plot on hypercubic lattices for $d_s = 3$, 4, and 5. The dashed line follows Eq. (10). The inset is for the plot of W as a function of t in $d_s = 3$, 4, and 5. The solid curve in the inset follows Eq. (11).

Next we discuss the simulation results of the CRSOS model on hypercubic lattices in $d_s=3$, 4, and 5. Here we have used the CD measure only. The early time behaviors of W(t)'s are shown in Fig. 6. The data for $d_s=3$ show a good straight line from the beginning, but the data for $d_s=4$ and 5 are curved all the time. From the relation $W(t) \sim t^{\beta}$ and the data for $\ln t > 3$, we have obtained

$$\beta \approx 0.08 \quad (d_s = 3) \tag{10}$$

and the fitted line corresponding to $\beta = 0.08$ for $d_s = 3$ is also shown in Fig. 6. It is hard to distinguish numerically between a logarithmic behavior and a power law behavior with a very small value of the power. A straight line fitting in $d_s = 4$ data in a log-log plot for $\ln t > 3$ gives $\beta \approx 0.02$. It is close to zero and the data are also well fitted by the curve

$$W(t) \simeq 0.015 \ln t$$
 (or $\beta = 0$) ($d_s = 4$) (11)

and this curve is also shown in Fig. 6. In other words, a good straight line can be obtained in a semilogarithmic plot. So we believe that the logarithmic behavior is more plausible. In the inset of Fig. 6, the $d_s = 5$ data show the saturation of the width after the initial transient times, implying that $d_s = 5$ is above the critical dimension. The result for $d_s = 4$ indicates that the upper critical substrate dimension d_s^c of the CRSOS model is 4. Since RG calculations [8,19] predict that d_s^c of Eq. (2) is 4, this result supports that the CRSOS model follows Eq. (2). The value of β from the simulation in $d_s = 3$ is smaller than $\beta_e = 1/11$. One possible explanation is that λ is renormalized such that there exists some correction in Eq. (7) like Janssen's correction [19] in addition to the effects of both the small system size and short simulation times.

We have investigated a conserved RSOS growth model in higher dimensions, where a dropped particle is allowed to hop to the nearest site satisfying the RSOS condition. The values of β and α are close to, but slightly smaller, than, those in Eq. (6) and the deviations in the values of α and β seem to be somewhat larger than Janssen's corrections. However, we have found that the CRSOS model has the upper critical substrate dimension $d_s^c = 4$ and the numerical value of $\alpha + z$ is close to but less than 4, consistent with Eq. (7). Considering the magnitudes of the estimated errors, the results for the CRSOS model do not exclude the values in Eq. (6). So we could not claim conclusively that our model breaks [19] the scaling relation $\alpha + z = 4$ due to the computer limitation. However, we find a consistent deviation of the exponents from Eq. (6). More larger simulations are required to find the corrections. On a square lattice, we have measured the surface width for both chemical distance measure and real distance measure. As one expected, the value of the exponent does not depend on the ways to define the distance. As a whole, the N=1 version of our CRSOS model in higher dimensions follows the continuum equation [Eq. (2)] well.

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