Surface morphology, hopping, and current in a conserved growth model with a restricted solid-on-solid condition

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A conserved growth model with a restricted solid-on-solid (RSOS) condition is described. A randomly dropped particle is allowed to hop to the nearest site satisfying the RSOS condition. The values of the dynamic exponents in the conserved growth model are consistent with those of the nonlinear equation $\partial h/\partial t = -\nu\nabla^4 h + \lambda\nabla^2(\nabla h)^2 + \eta$, where η is a random noise. The surface current measurement shows the absence of the Edwards-Wilkinson-type diffusion term. The surfaces in the steady-state regime have a grooved phase characterized by the roughness exponent $\alpha = 1$. The physical origin of the conserved nonlinear term is also discussed. [S1063-651X(97)15903-7]

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I. INTRODUCTION

There have been considerable efforts in the study of various growth models [1]. Since the surface structures of many growth processes are self-affine, most studies have concentrated on the surface width W, which is defined as the root mean square fluctuation of the surface height. In a finite system of lateral size L, the width W starting from a flat substrate scales as [1]

$$W(t) \sim L^\alpha f(t/L^z) \sim t^\beta, \quad t \ll L^z \sim L^\alpha, \quad t \gg L^z, \quad (1)$$

where the scaling function $f(x)$ is x^β for $x \ll 1$ and constant for $x \gg 1$. The exponents β and z are connected with the relation $z = \alpha/\beta$. Among them, the class of models known as solid-on-solid (SOS) models have been extensively studied as simple models of both equilibrium and nonequilibrium properties of surfaces. The characteristic feature of SOS models is the restriction of fluctuations to exclude overhangs and lattice vacancies. An important variation among the SOS models is the restricted SOS (RSOS) model, in which the differences between neighboring heights of the local columns $|\delta h|$ are usually restricted to zero or unity in magnitude. Even with this restriction, the equilibrium RSOS model still exhibits a roughening transition at three dimensions [2]. The nonequilibrium growth model with the RSOS condition [3] is also well described by the Kardar-Parisi-Zhang (KPZ) equation [4–6].

Recently, there have been some studies in ‘‘conserved growth models’’ [7–16] to find the possible relevance of these models to the real molecular beam epitaxial (MBE) growth. In these models the number of particles is conserved after being deposited, whereas the number of particles is not conserved in the simple RSOS growth model [3]. One of the major issues in the studies is to find the universality class of various atomistic growth (or MBE) processes. It has been suggested [8,9] that some atomistic models for MBE growth may belong to the conserved KPZ universality class [7,8,16], which is different from the KPZ class [4]. Even though there are some recent experimental evidences [14] supporting this claim, the issue is still quite controversial. It would, therefore, be helpful if one can construct alternate models which belong to the conserved KPZ class. The so-called ‘‘conserved growth models’’ have the distinguished feature that the dropped particle is allowed to hop along the surface without desorption. So far, there is no firm understanding between discrete growth models and a nonlinear conserved continuum equation [7,8,13].

Here, we study a conserved growth model with the RSOS condition [15] in detail. We find that our model follows a nonlinear MBE growth equation of Lai and Das Sarma [7] and Villain [10],

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

where $h(x,t)$ is the height of the film and η is a *nonconserved* Gaussian random noise satisfying

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

The one-loop renormalization group (RG) calculation [7] for Eq. (2) gives $\alpha = (5-d)/3$ and $z = (7+d)/3$, i.e., $\beta = (5-d)/(7+d)$. In $d = 1+1$, $\beta = 1/3$ is the same as the value of KPZ exponent, but $z = 3$ is different from $z_{\mathrm{KPZ}} = 3/2$. Sun, Guo, and Grant [16] studied Eq. (2) with *conserved noise* by one-loop RG calculation and found different values $\beta = 1/11$ and $z = 11/3$ in $d = 1+1$. Racz *et al.* [17] studied various atomistic models with *conserved noise* and related some of their discrete models to Eq. (2) with *conserved noise*. There have been some physical explanation for the nonlinear term [10].

To claim that our conserved model follows Eq. (2) exactly, we investigate the scaling property (or the values of the exponents), the hopping distance of particles along the

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surface, the surface current, and the morphology of the surface in the steady-state regime. Our study is done mainly in $d=1+1$. The outline of this paper is as follows. In Sec. II our model is described in detail, and the scaling properties of the surface width in the model are given. Then the hopping distances of particles along the surface are discussed in Sec. III. Section IV contains the tilt-dependent surface current measurements. In Sec.V, the morphologies of the steady-state surfaces are studied. Finally in Sec. VI, discussions and conclusions are given.

II. UNIVERSALITY CLASS OF THE CONSERVED RSOS MODEL

We now describe a conserved growth model with the RSOS condition. The growth algorithm of the model is very similar to the simple RSOS growth model [3] except no desorption. The growth rule is following: (i) A site $\vec{x}$ is selected randomly on $(d-1)$-dimensional substrate. (ii) If the restricted solid on solid condition (RSOSC) 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 RSOSC is not obeyed at the position $\vec{x}$, the dropped particle is allowed to hop to the nearest site to $\vec{x}$ where the RSOSC is satisfied. If there are more than one neighboring site at the same distance from $\vec{x}$ which satisfies the RSOS condition, one of them is chosen randomly with equal probability.

In the simple RSOS growth model [3], a site on a $d-1$-dimensional substrate is randomly selected, and the growth is permitted on the selected site provided the nearest neighbor height difference is not larger than the restriction parameter N. If the RSOSC is not satisfied, then the dropped particle is rejected. However, our model allows the dropped particle to hop to the nearest site where the RSOSC is satisfied. So our model is rejection free, and our model faithfully produces a RSOS model with the constraint of conserved particle growth. To find a site satisfying RSOSC, the dropped particle can hop both up and down directions along the surface. The simple RSOS growth model [3] allows a desorption of the dropped particles, and produces the KPZ nonlinear term [4]. In our conserved model, since the dropped particle is allowed to hop both in the up and down directions, there is no surface diffusion term of Edwards and Wilkinson model [18]. (In Sec. IV we show it by measuring the tilt-dependent surface current.) Instead, there may be a conserved nonlinear term due to the RSOS restriction.

The universality class of a growth model is determined by the values of the dynamic exponents α and β (or z). Our simulations are performed in $d=1+1$ from a flat substrate with periodic boundary conditions. The simulations are typically done for the restriction parameters $N=1$ and 2 [19]. The time t corresponds to the number of Monte Carlo steps (number of layers). To determine the growth exponent β, we measure $W(t)$ as a function of time for a system size $L=10\,000$, averaging over 60 independent runs in $d=1+1$. Through the relation $W(t)\sim t^{\beta}$ for early times $t\ll L^{z}$, we obtain

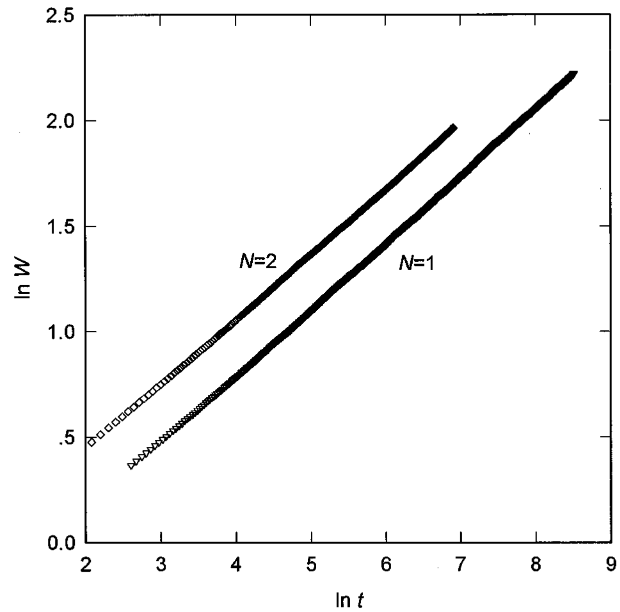

FIG. 1. Surface width W as a function of time in log-log plot for both $N=1$ and 2 ($L=10\,000$ and $d=1+1$).

$$\beta=0.32\pm0.01 \quad (d=1+1). \tag{4}$$

As shown in Fig. 1 the value of β remains the same within the error for both $N=1$ and 2. For the roughness exponent α describing the saturation of the interface fluctuation, we use the relation $W(t)\sim L^{\alpha}$ for the system size L in the steady-state regime $t\gg L^{z}$. We have used system sizes $L=64$, 90, 128, 180, and 256. From the data shown in Fig. 2, we obtain

$$\alpha=0.95\pm0.04 \quad (d=1+1). \tag{5}$$

The value of α also remains the same within the error for both $N=1$ and 2. Through the relation $z=\alpha/\beta$, we obtain

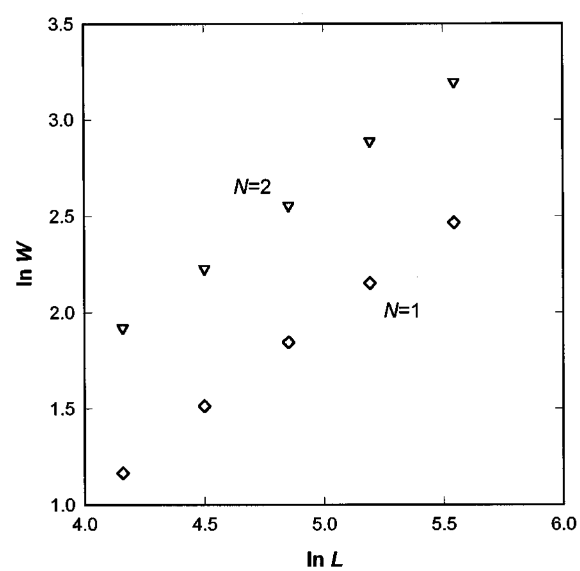

FIG. 2. Saturated surface width W as a function of L in log-log plot for both $N=1$ and 2.

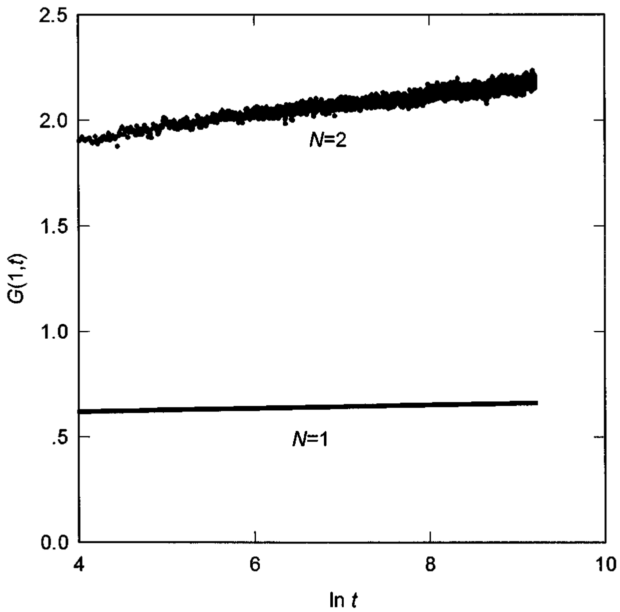

FIG. 3. $G(1,t)$ as a function of time in semilog plot for both $N=1$ and 2 $(d=1+1)$.

$\approx 0.95/0.32 \approx 2.97$ in $d=1+1$. These exponents of our model are in very good agreement with $\beta=\frac{1}{3}$, $\alpha=1$, and $z=3$ obtained analytically from Eq. (2) in Ref. [7]. They also satisfy the scaling relations [7,8,16]

$$z-2\alpha-d+1=0, \tag{6}$$

$$z+\alpha=4 \tag{7}$$

very well. The scaling relation of Eq. (6) is due to the conservation of the number of particles after being dropped [8]. Another interesting quantity is the correlation function $G(r,t)=\langle(h(x+r,t)-h(x,t))^2\rangle$. As explained in Refs. [20,21,23], if $\alpha>1$, $G(1,t)$ grows as t^{γ} for small t with $\gamma=2(\alpha-1)/z$ in $d=1+1$. In our model, γ is expected to be zero so that $G(1,t)$ grows as $\ln t$ in $d=1+1$. We have confirmed numerically that the plot of $G(1,t)$ versus $\ln t$ shows a straight line for both $N=1$ and 2 as shown in Fig. 3. All these results involving surface width and correlation function support our assertion that our model belongs to the same universality class as Eq. (2).

III. DISTRIBUTION OF HOPPING DISTANCES

There exist some other conserved growth models [8,9,13] as well. Wolf and Villain (WV) model [8] and Das Sarma and Tamborenea (DT) model [9] allow a dropped particle to hop to maximum bond sites. In DT and WV models, there exists a finite vertical diffusion due to possible high steps. Similarly in our model, there may be a long distance hopping of a dropped particle to find a site where the RSOSC is satisfied. If the chance for a particle to hop in a long distance (or in a distance comparable to the size of a substrate) is high, then our model should have nonlocal processes. So, we measure the probability distribution $P(l)$ as a function of l where l is the hopping distance between the dropped site (the selected site) and the deposited site (the nearest site which satisfies the RSOSC). If the dropped site satisfies the RSOSC, the particle does not move with $l=0$. We have measured $P(l)$ for the restriction parameters $N=1$ and 2. By monitoring the hopping distances of three million dropped particles at the steady-state regime for the system sizes $L=128$, 256, and 512 over 30 independent runs, we have obtained $P(l)$'s, which is shown in Fig. 4. The data for both $N=1$ and 2 are well fitted to exponential distributions as

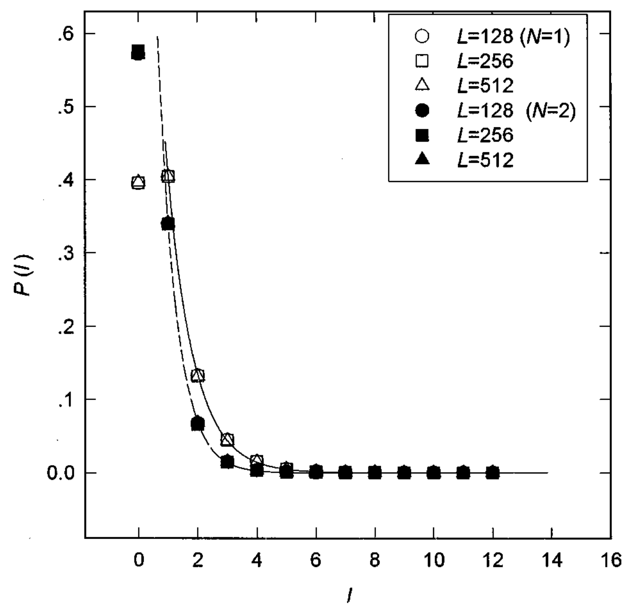

FIG. 4. Measured probability distributions $[P(l)\text{'s}]$ of hopping distances (l) in the steady-state regime for $N=1$ and 2, and for the system sizes $L=128$, 256, and 512. The solid curve is an exponential fit to data for $N=1$ and the dotted curve is such a fit for $N=2$ [see Eq. (8)].

$$P(l)=A\exp(-l/l_r),$$

$$(A=1.23, \quad l_r=0.90 \quad \text{for } N=1$$

$$A=1.69, \quad l_r=0.62 \quad \text{for } N=2) \tag{8}$$

except the points of $l=0$. We have also calculated average hopping distance $\langle l\rangle=\Sigma_l lP(l)$ and obtained $\langle l\rangle=0.91$ for $N=1$ and $\langle l\rangle=0.56$ for $N=2$. The average hopping distances for the system sizes $L=128$, 256, and 512 are almost the same for the given N. We find that $P(l)$'s follow exponential distributions regardless of the values of N, whereas the average hopping distance decreases as N increases. In principle, it is possible for a particle to have a very long hopping distance, but such an event happens with very rare probability, as you can see in Fig. 4. Since measured $P(l)$'s for various system sizes satisfy an exponential decay quite well, the distributions do not have a long-ranged tail which can be seen in a power-law distribution. We conclude that the basic growth process in the conserved RSOS growth model is a local process.

IV. SURFACE CURRENT

The WV model [8] allows only downward jumps, so that the surface current probably producing nonzero diffusion

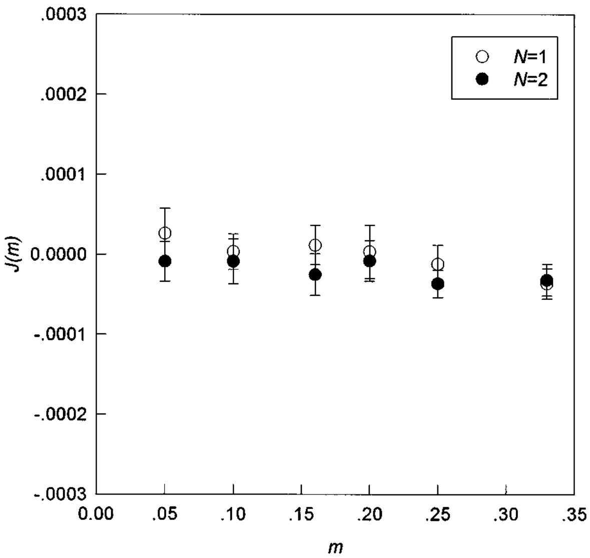

FIG. 5. Surface currents $J(m)$ in the steady-state regime for $N=1$ and 2, where m is the slope of the substrate.

characteristics of the Edwards and Wilkinson (EW) model [18]. The diffusion term generates the on average downward movement of the dropped particles. If a surface growth model has a characteristic of the diffusion, then the corresponding continuum equation can be described by

$$\frac{\partial h(x,t)}{\partial t} = \nu_2 \nabla^2 h(x,t) + [\text{other } h(x,t) \text{ dependent terms}] + \eta. \quad (9)$$

Recently Krug, Plischke, and Siegert [22] have suggested a method to determine the surface diffusion coefficient ν_2 in various growth models by measuring the surface current $J(m)$ as a function of m, which is the average slope of the tilted substrate. The surface current is measured by counting the number of jumps in between the uphill and downhill directions. If a net current is in uphill direction, $J(m)$ is positive. ν_2 can be given $\nu_2 = -(\partial J/\partial m)(m=0)$. The tilt-dependent current analysis [22] shows that the WV model belongs to the EW [18] universality class [23]. If there is a very small negative current, the crossover behavior to EW class will be very slow. Since a dropped particle is allowed to hop equally in both up and down directions in our model, we expect there is no surface diffusion term. To show this explicitly, we measure the surface current $J(m)$ as a function of the surface tilt parameter m. We do not consider the length of the jump; instead, we just count the number of the particles which hop to downhill (or uphill) jump. The currents are taken in the steady-state regime for the system size $L=512$ and for the restriction parameter $N=1$ and 2. As shown in Fig. 5, the $J(m)$ is very small (or less than 10^{-4}) and is almost independent of m for both $N=1$ and 2. Thus the diffusion coefficient $\nu_2 = -J'(0)$ is nearly equal to zero. Therefore we hardly expect that there is a crossover to the EW class in our model.

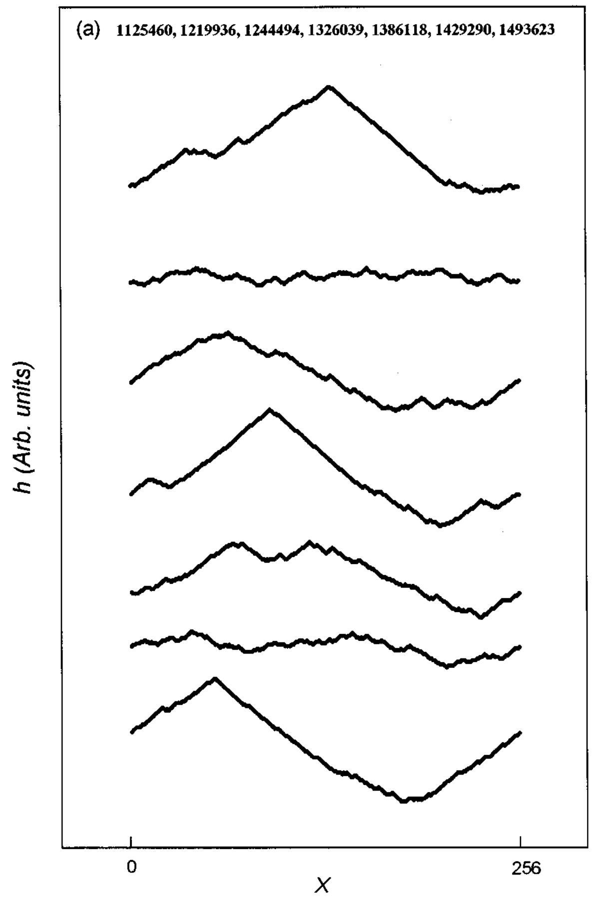

FIG. 6. (a) Typical surface configurations in the steady-state regime in one simulation for the system size $L=256$ and (b) those in another simulation. The numbers in the top of the figures denote the Monte Carlo times at which each surface configuration is taken. The configurations of the earlier times come nearer to the bottom of the figures.

V. SURFACE MORPHOLOGY AT THE STEADY-STATE REGIME

To understand the relation of our model to Eq. (2) more deeply, we have investigated the surface morphologies of the conserved growth model with the RSOSC in the steady-state regime. Figures 6(a) and 6(b) have some typical surface configurations of our model at the steady-state regime for the system size $L=256$. The surface patterns in Fig. 6(a) are taken for t between 10^6 and 1.5×10^6 in one simulation, and those in Fig. 6(b) are taken for t between 6×10^6 and 7×10^6 in another simulation. From both Figs. 6(a) and 6(b) one can infer that the grooved phases of growing surfaces occur frequently and disappear at the steady-state regime. Such grooved phases last for a considerable time interval, before rather flat patterns are formed. In contrast, for the simple RSOS growth model the surfaces behaves like a random walk in $d=1+1$, producing $\alpha=\frac{1}{2}$. The grooved phases characterized by the rougheness exponent $\alpha=1$ appears to be the deterministic (noise-free) steady-state solution of Eq. (2) [17]:

$$h(x) = h_0 + c_1 \ln[\cosh\{c_2(x-x_o)\}], \quad (10)$$

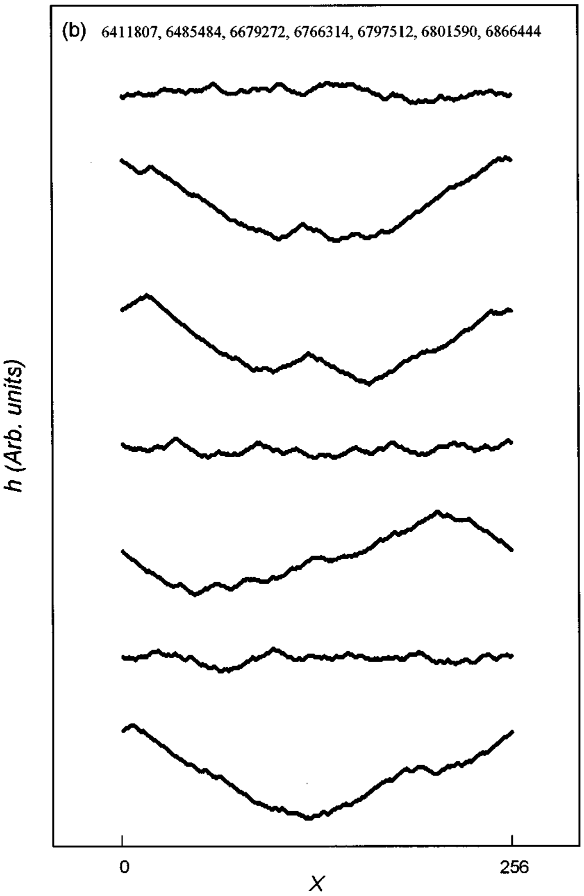

FIG. 6 (*Continued*).

where x_o, h_o, c_1, and c_2 are constants. Through numerical fits, we have confirmed that the grooved phases in Figs. 6(a) and 6(b) are consistent with Eq. (10). Racz et al. [17] also found such grooved phases in the critical and decisive analysis of the Sun, Guo and Grant's [16] noise-conserved stochastic model. The grooved phase in our model has a sharp peak and a round valley. The surface configurations also reflect the broken $h \rightarrow -h$ symmetry of Eq. (2). The analysis for the steady-state surfaces based on Fig. 6 also provide an identification that our model follows Eq. (2).

VI. DISCUSSIONS AND CONCLUSIONS

We can rewrite Eq. (2) as $\partial h/\partial t = -\nabla \cdot \mathbf{J} + \eta$ with the surface current **J**,

$$\mathbf{J} = \nabla[\nu \nabla^2 h - \lambda (\nabla h)^2]. \qquad (11)$$

Since the dropped particle on a sloped region hops to flat area, surface current is generated from the higher sloped region to the lower sloped region. Thus we can argue that our model has a positive λ in Eq. (2) [13]. This is the reason why the conserved growth with a RSOSC produces the nonlinear effect. It is interesting that the nonconserved RSOS growth model [3] generates the KPZ nonlinearity, and the conserved growth model with RSOSC produces the conserved nonlinearity in Eq. (11). The sign of λ is irrelevant, so it might be interesting to construct a model having a negative λ which belongs to the same universality class. There is a different model [11] having a similar value of exponent β, where Arrhenius hopping is allowed in SOS model. Since a kink site is more favorable than a single bond site in the model, it may have negative λ [13]. The different signs of λ between our model and Ref. [11] is probably due to the different physical origin [24]. In our model, it is hard to stick to the vicinal surface. However, a kink site is more favorable in other model. It is not exactly known whether the model [11] follows Eq. (2) or not. The similar behavior in KPZ equation is also shown in the finite temperature RSOS growth model, where the KPZ nonlinearity depends on a temperaturelike parameter [24]. In realistic growth, the dropped particle may hop quite a long distance at high temperature to prevent a high step, and then the surface configuration in real crystal growth may satisfy the RSOS condition.

In conclusion, we have introduced a simple conserved growth model with the RSOS condition which follows the nonlinear equation (2). The numerical study of the models shows that dynamical exponents (or scaling property), the morphology of the surfaces at the steady-state regime, and the property of hoppings are in good agreement with the theoretical results of the continuum equation. The measurement of the tilt dependent surface current supports that the EW-type diffusion term is absent in the model. The conserved growth with the RSOS condition effectively produces the conserved nonlinear term in Eq. (2). The relation between the MBE growth and our model remains to be understood.

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