Scaling of rough surfaces with nonlinear diffusion

Takashi Nagatani

College of Engineering, Shizuoka University, Hamamatsu 432, Japan

(Received 27 November 1990)

Surface properties of a random-deposition model that includes the effects of surface diffusion with nonlinear diffusivity are studied in $1+1$ dimensions. The nonlinear diffusivity $D(h)$ obeys a power law h^k . For a sufficiently large deposit, the variation of the surface thickness with the height of deposit shows anomalous behavior for the power k . It is found that the exponent β , describing how the surface thickness grows with the height, is given by $\beta=(1-k)/4 < 0$ (for $k > 1$), $\beta=0$ (for $k=1$), $\beta=(1-k)/4 > 0$ (for $1 > k > 0$), $\beta=\frac{1}{4}$ (for $k=0$; linear diffusion), and $\beta=\frac{1}{2}$ (for $k < 0$). The case of $k=1$ is a marginal state, and the surface thickness approaches a constant value with increasing height.

I. INTRODUCTION

Surface structures of growth processes have recently attracted considerable attention.¹ Much of this interest stems from the fact that in addition to their connection to processes of fundamental practical importance, such as thin-film growth and interface dynamics in random media, these models exhibit nontrivial scaling behavior. For the ballistic deposition model,² the Eden model,³ and the random deposition model with surface diffusion,⁴ it has been shown that the surface of the deposit exhibits a self-affine fractal geometry that can be described in terms of the scaling form

$$\xi = L^\alpha f(h/L^z), \quad (1)$$

where ξ is the variance of the surface height, h is the mean height of the deposit, and L is the lateral size of the deposit. The scaling function $f(x)$ tends to a constant value when x tends to infinity and behaves as x^β when x tends to zero. ξ behaves as L^α for large h and as h^β for large L . In $1+1$ dimensions, simulations give α equal to $\frac{1}{2}$ and β about $\frac{1}{3}$ for the ballistic model^{2,5} and the Eden model.^{3,6} By introducing surface diffusion in the random deposition model,⁴ it has been found that the value of the β exponent becomes $\frac{1}{4}$. Also it has been shown that the same value of the β exponent is obtained when surface diffusion or complete restructuring⁷ is included in the ballistic deposition model.

A theory of deposition processes by Edwards and Wilkinson⁸ is able to predict the values of α, β, z for the random-filling model with surface diffusion. By solving a linear Langevin equation for the growing surface, they derived the exponents

$$\alpha=(2-d)/2, \quad \beta=(2-d)/4, \quad z=2 \quad (2)$$

in $d+1$ dimensions, where d is the dimension of the substrate. In $1+1$ dimensions, the result $\alpha=\frac{1}{2}$, $\beta=\frac{1}{4}$, and $z=2$ are in excellent agreement with simulations.⁴ For ballistic deposition with surface restructuring, $(2+1)$ -dimensional simulations of the off-lattice process indicate

that the surface width diverges logarithmically with h and L in better agreement with the theoretical result $d_c=2$ [Eq. (2)].⁹ This work was later extended by Kardar, Parisi, and Zhang,¹⁰ who took into account the possibility of lateral growth. They showed that the exponents become $\alpha=\frac{1}{2}$, $\beta=\frac{1}{3}$, and $z=\frac{3}{2}$ in $1+1$ dimensions. It appears the result $\beta=\frac{1}{4}$ for deposition models with restructuring can be accounted for by a theory of Edwards and Wilkinson, while the value of β for a ballistic model without restructuring, $\beta=\frac{1}{3}$, can be accounted for by a theory of Kardar, Parisi, and Zhang. The dynamics of the interface in these models has been shown to be intimately related to a variety of other problems, including directed polymers in random media, the large-time behavior of randomly stirred fluids, and the evolution of Sivashinski flame fronts.¹¹⁻¹³

Jullien and Meakin¹⁴ also studied the influence of a finite concentration of falling particles in ballistic deposition with restructuring in $1+1$ dimensions. They found that the exponent β for an extremely large deposit varies from $\frac{1}{4}$ (for small concentrations) to $\frac{1}{3}$ (for large concentrations). Krug¹⁵ proposed a classification of deposition processes that explains why some models are governed by the linear theory.⁸

Using dynamic renormalization-group techniques, Kardar, Parisi, and Zhang¹⁰ pointed out that $d=2$ (in $d+1$ dimensions) must be a critical dimension above which the scaling of the stochastic Burgers equation should change. Halpin-Healy,¹⁶ using a functional renormalization-group method, was able to make some more precise predictions. He showed that there exists an upper critical dimension $d=4$, above which all exponents follow their mean-field values, while for $d < 2$ the strong-coupling phase prevails. For $2 < d < 4$, there should be a phase transition between the strong-coupling and the weak-coupling phases.

Very recently, Amar and Family¹⁷ found a phase transition in a restricted solid-on-solid surface-growth model in $2+1$ dimensions. It is shown that the phase transition is not due to a nonequilibrium analog of a roughening transition, but to the vanishing of the coefficient of the

nonlinear term in the Kardar-Parisi-Zhang equation of a growing interface.^{18,19} Yan, Kessler, and Sander²⁰ and Pellegrini and Jullien²¹ also found by computer simulations that a roughening phase transition in surface growth occurs in both 2+1 and 3+1 dimensions. They introduced simple ballistic models for surface growth that consider a probability of sticking or sliding, or a mixture of sticky and sliding particles. The models are believed to be discrete versions of the stochastic Burgers equation.

In this paper we consider the effects of nonlinear surface diffusion on the scaling structure of surface properties in the random-filling deposition model in 1+1 dimensions. We assume that the diffusivity $D(h)$ behaves as a power law h^k . The growth of an interface from a substrate can be described by

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left[h^k \frac{\partial h}{\partial x} \right] + \eta(x, t), \quad (3)$$

where $h(x, t)$ is the height of the interface at position x and time t , and $\eta(x, t)$ is white noise in space and time. In the limit $k \rightarrow 0$, Eq. (3) reduces to the linear equation of Edwards and Wilkinson.⁸ For $k > 0$, the surface diffusion becomes stronger with increasing height; the surface roughness will be weakened and the exponent β will become smaller than the value $\frac{1}{4}$ predicted by the theory of Edward and Wilkinson. With large k , the surface diffusion will suppress the surface roughness with increasing height. Then the surface roughness may decrease with increasing height. Thus we expect that a roughness transition occurs with increasing power k . The exponent β will change from a positive value through zero to a negative value with increasing power k . On the other hand, for $k < 0$, the surface diffusion becomes weaker with increasing height. The surface roughness will be intensified and the exponent β will approach the

value $\frac{1}{2}$ of the random-filling model.

We introduce the power k to extend the linear equation to the nonlinear equation. As k varies, we expect that the roughness transition will appear even in 1+1 dimensions, a case for which it is easy to perform the computer simulation.

II. MODEL

We introduce a rough-surface model with nonlinear surface diffusion. We assume the surface diffusivity $D(h)$ behaves as a power law h^k . We investigate the effects of nonlinear surface diffusion on the scaling structure of surface properties in the random-filling deposition model in 1+1 dimensions. This model is an extended version of the random deposition model with linear surface diffusion devised by Family.⁴ The growth of an interface from a substrate is described by Eq. (3). The nonlinear diffusion equation (3) has a large number of applications and has been investigated by mathematicians. Unfortunately, the rough surfaces governed by nonlinear surface diffusion have not been found in thin-film experiments. However, physical realizations of a rough surface governed by nonlinear surface diffusion are possible. Here we consider such a physical realization. We assume that there is a negative temperature gradient normal to the substrate. The diffusivity is generally dependent upon the temperature, increasing as temperature increases. Then the surface diffusivity increases with increasing height. The growth process of thin films is controlled by this surface diffusion with height-dependent diffusivity. The interface dynamics of the growth process can be described by Eq. (3).

We derive the difference equation of the nonlinear diffusion equation (3) for computer simulations. The difference equation is given by

$$h(x, t+1) = \begin{cases} h(x, t) + \eta(x, t) + \frac{1}{R} [h(x, t)/L]^k [h(x+1, t) + h(x-1, t) - 2h(x, t)], & k > 0 \\ h(x, t) + \eta(x, t) + \frac{1}{R} h(x, t)^k [h(x+1, t) + h(x-1, t) - 2h(x, t)], & k \leq 0 \end{cases} \quad (4)$$

where L is the system size and R is the constant value to guarantee the convergence of the difference equation. For $k > 0$ the diffusivity must be less than unity. We normalized the diffusivity as $[h(x, t)/L]^k$ for $k > 0$. In the original random-filling model, particles are added randomly, one at a time, onto a growing surface following linear trajectories and sticking on the top. The dynamics for deposition orthogonal to the substrate follows the equation

$$h(x, t+1) = h(x, t) + 1. \quad (5)$$

In our simulations, we allow particles to diffuse by implementing an additional term, which changes (5) to

$$h(x, t+1) = \begin{cases} h(x, t) + 1 + \frac{1}{R} [h(x, t)/L]^k [h(x+1, t) + h(x-1, t) - 2h(x, t)], & k > 0 \\ h(x, t) + 1 + \frac{1}{R} h(x, t)^k [h(x+1, t) + h(x-1, t) - 2h(x, t)], & k \leq 0. \end{cases} \quad (6)$$

Equation (6) is derived from Eq. (5) by taking into account Eq. (4). In our simulations, nonlinear surface diffusion occurs simultaneously with the deposition.

Our simulations are performed on a flat-line-lattice substrate in $1+1$ dimensions. Periodic boundary conditions in the lateral direction are used throughout the simulation. In our work, we attempt to get accurate values of the scaling exponent β describing how the surface thickness increases with the height for an extremely large deposit. We cannot perform the simulations for the scaling exponent α since the diffusivity $D(h)$ must have an upper bound for the height. Here we are interested in the emergence of the roughness transition, which can be distinguished by the change of the exponent β from a positive value through zero to a negative value. This roughness transition has been predicted by the theory of Edwards and Wilkinson⁸ but has only been found in the works of Yan, Kessler, and Sander²⁰ and Pellegriani and Jullien.²¹

III. RESULTS AND SUMMARY

We performed computer simulations for $L = 5000$. In Figs. 1 and 2, we show log-log plots of the surface thickness ξ against the height for $k = -2, -1, 0, 0.5, 1, 1.5$, and 2. The height is defined by its mean value, while the surface thickness is defined by its variance. We set the constant $R = 3$ and $R = 27$, respectively, in Figs. 1 and 2. With $R = 3$ (Fig. 1), the surface thickness begins to diverge at $h = 150$ for $k = 0$, and at $h = 700$ for $k = 0.5$. With $R = 27$ (Fig. 2), the surface thickness converges for all k until the height h reaches 1000. We find that the surface thickness approaches a constant value with increasing height for $k = 1$. For $k > 1$, the surface thickness reaches a maximum value and then decreases with

FIG. 1. Surface thickness ξ as a function of the mean height h of the deposit (log-log plot) for $k = -2, -1, 0, 0.5, 1$, and 2 with $R = \frac{1}{3}$. For $k < 0$, the slope is $\frac{1}{2}$. For $k = 0$ (linear diffusion), the slope is $\frac{1}{4}$ until $h = 150$. For $k = 1$, the slope approaches a constant value. For $k > 1$, the slope is initially $\frac{1}{2}$, then the surface thickness reaches a maximum value, and decreases with increasing height.

FIG. 2. Surface thickness ξ as a function of the mean height h (log-log plot) for $k = -2, -1, 0, 0.5, 1$, and 1.5 with $R = \frac{1}{27}$. For $k = 0$ (linear diffusion), the slope is $\frac{1}{4}$ until $h = 1000$. For all k , the surface thickness converges until $h = 1000$.

growing height. The case of $k = 1$ is a marginal state. For $k = 0$ the slope of the surface thickness against the height equals $\frac{1}{4}$. This corresponds to the linear surface diffusion. For $k < 0$, the slope of the surface thickness against the height is $\frac{1}{2}$. This is consistent with the exponent of random-filling deposition. For $k < 0$, the surface diffusion becomes negligible. We show the dependence of the slope of the surface thickness on the height for various nonlinearity powers k in Fig. 3 ($0 < k < 1$) and in Fig. 4 ($k > 1$) in log-log plots. In Fig. 3, we set $R = \frac{1}{27}$ to guarantee the convergence of Eq. (6) before $h = 1000$. In Fig. 4, we set $R = \frac{1}{3}$ to guarantee the convergence before $h = 1000$. We draw the line $(1-k)/4$ for each curve. We find the exponent β to equal $(1-k)/4$ for $k > 0$. Thus we show the roughness transition occurring at $k = 1$. The results obtained are summarized as follows. The surface thickness satisfies the following relation:

FIG. 3. For $0 < k < 1$, the dependence of the slope of the surface thickness on the height for various values of the nonlinearity power of k . The straight line with the slope $(1-k)/4$ is drawn for each curve ($k = 0, 0.2, 0.4, 0.6, 0.8$, and 1).

FIG. 4. For $k > 1$, the dependence of the slope of the surface thickness on the height for various values of the nonlinearity power k . The straight line with the slope $(1-k)/4$ is drawn for each curve ($k = 1.25, 1.5, 1.75, 2$, and 2.25).

$$\xi \approx h^{(1-k)/4} \text{ for } 0 < k < 1 \text{ and } 1 \ll h \ll L. \quad (7)$$

For $k=1$, the surface thickness approaches a constant value with increasing height

$$\xi = \text{const} \text{ for } k=1 \text{ and } 1 \ll h \ll L. \quad (8)$$

For $k > 1$, the surface thickness first increases with increasing height (the exponent $\beta = \frac{1}{2}$), reaches a maximum value, and then decreases with the exponent $\beta = (1-k)/4 < 0$. The surface thickness crosses over from random-filling deposition to strong surface diffusion. The surface thickness satisfies the following relation:

$$\xi \approx h^{(1-k)/4} \text{ for } k > 1 \text{ and } h_c < h \ll L, \quad (9)$$

where h_c is the crossover length from random-filling deposition to strong diffusion. For $k < 0$, the surface diffusion is weakened with increasing height. The surface thickness satisfies the following relation:

$$\xi \approx h^{1/2} \text{ for } k < 0 \text{ and } 1 \ll h \ll L. \quad (10)$$

This is consistent with the scaling relation of the random-filling deposition without surface diffusion. For $k < 0$, the surface diffusion becomes much weaker with increasing height, and the surface diffusion becomes negligible.

In summary, we present a random deposition model that takes into account the effects of nonlinear surface diffusion. We introduce the power k of the nonlinearity to replace the dimension d . We study how the surface roughness varies with k in $1+1$ dimensions. We found that the exponent β is given by $\beta < 0$ for $k > 1$, $\beta = 0$ for $k = 1$, $\beta > 0$ for $0 < k < 1$, $\beta = \frac{1}{4}$ for $k = 0$, and $\beta = \frac{1}{2}$ for $k < 0$. The case of $k = 1$ is a marginal state at which the roughness transition from $\beta > 0$ to $\beta < 0$ occurs.

¹T. Vicsek, *Fractal Growth Phenomena* (World Scientific, Singapore, 1989).

²F. Family and T. Vicsek, *J. Phys. A* **18**, L75 (1985).

³R. Jullien and R. Botet, *J. Phys. A* **18**, 2279 (1985).

⁴F. Family, *J. Phys. A* **19**, L441 (1986).

⁵P. Meakin, P. Ramanlal, L. M. Sander, and R. C. Ball, *Phys. Rev. A* **34**, 5081 (1986).

⁶P. Meakin, R. Jullien, and R. Botet, *Europhys. Lett.* **1**, 609 (1986).

⁷P. Meakin and R. Jullien, *J. Phys. (Paris)* **48**, 1651 (1987).

⁸S. F. Edwards and D. R. Wilkinson, *Proc. R. Soc. London Ser. A* **381**, 17 (1982).

⁹R. Jullien and P. Meakin, *Europhys. Lett.* **4**, 1385 (1987).

¹⁰M. Kardar, G. Parisi, and Y. C. Zhang, *Phys. Rev. Lett.* **56**, 889 (1986).

¹¹D. Forster, D. R. Nelson, and M. J. Stephen, *Phys. Rev. A* **16**,

732 (1977).

¹²E. Medina, T. Hwa, M. Kardar, and Y. Zhang, *Phys. Rev. A* **39**, 3053 (1989).

¹³J. Cook and B. Derrida, *J. Stat. Phys.* **57**, 89 (1989).

¹⁴R. Jullien and P. Meakin, *J. Phys. A* **22**, L219 (1989).

¹⁵J. Krug, *J. Phys. A* **22**, L769 (1989).

¹⁶T. Halpin-Healy, *Phys. Rev. Lett.* **62**, 442 (1989).

¹⁷J. G. Amar and F. Family, *Phys. Rev. Lett.* **64**, 543 (1990).

¹⁸J. Krug and H. Spohn, *Phys. Rev. Lett.* **64**, 2332 (1990).

¹⁹J. Kim, Tapio Ala-Nissila, and J. M. Kosterlitz, *Phys. Rev. Lett.* **64**, 2333 (1990).

²⁰H. Yan, D. Kessler, and L. M. Sander, *Phys. Rev. Lett.* **64**, 926 (1990).

²¹Y. P. Pellegrini and R. Jullien, *Phys. Rev. Lett.* **64**, 1745 (1990).