Nonequilibrium roughening transition in an interface growth model with two species of particles

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We introduce an interface growth model exhibiting a roughening transition from a smooth to a rough phase, related to a nonequilibrium phase transition (NPT) from an active to an inactive phase at the bottom layer. In the model, two different species of particles are deposited or evaporated, and a dynamic rule is assigned symmetrically or asymmetrically with respect to particle species. It is found that for the asymmetric case, the roughening transition and the NPT belong to the directed percolation universality class, while for the symmetric case, they are related to the directed Ising universality class. $\left[S1063-651X(99)01811-5 \right]$

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Recently the roughening transition (RT) from a smooth to a rough phase in nonequilibrium systems has attracted considerable interest in physical literature $[1]$. The RT in nonequilibrium systems occurs even in one dimension, which might be interpreted as a spontaneous symmetry breaking phenomenon of a nonconserved order parameter $[2,3]$. The examples of the RT include the deposition-evaporation (DE) model with no evaporation on terrace $[2]$, the fungal growth model $[3]$, the polynuclear growth model $[4]$, etc. The common feature of the RT in the above models is that the RT is related to directed percolation (DP) [5]. The reason is that each of the interface models contains a reference height where the nonequilibrium phase transition (NPT) from an active to an inactive state occurs, which belongs to the DP universality class: When the site where the interface touches the reference height is called vacant site, the density of the vacant site exhibits the NPT from being finite (active state) to decaying to zero exponentially (inactive state). In the active state, the interface is smooth, while in the inactive state, it is rough. Thus, the RT occurs at the same critical point of the NPT, and is characterized by the universal property of the NPT. For example, the reference height of the DE model is the bottom layer, on which the NPT belongs to the DP universality class. Thus, the RT in the DE model is related to DP.

It has been shown that the NPT is classified according to the number of equivalent inactive states $[6]$. The inactive state means the configuration with frozen dynamics. The NPT with one inactive state belongs to the DP universality class, of which the examples include the monomer-dimer model for the catalytic oxidation of CO $[7]$, the contact process $[8]$, the surface depinning model $[9]$, the branchannihilation random walks with odd numbers of offspring $[10]$, etc. When two inactive states exist, the NPT belongs to the directed Ising (DI) universality class, equivalent to the class of parity-conserving branching-annihilation random walks $[10]$. The examples include the probabilistic cellular automata model $[11]$, the kinetic Ising model $[12]$, the interacting monomer-dimer model $[13]$, the modified Domany-Kinzel model $[14]$, etc.

The interface models $[2-4]$, however, do not contain any inactive state, and the dynamics proceeds without being trapped, even though their monolayer version contains inactive state. Thus, it would be interesting to find the way how to classify the universality class for the RT. In this paper, we propose that the number of the symmetric state lying in the dynamic rule plays the role of classifying the universality class for the RT. In order to confirm this, we introduce a stochastic interface model with twofold symmetry, and compare it with its asymmetric version. It is found that the RT for the two cases behave differently from each other, and the symmetry in the dynamic rule indeed classifies the universality class of the RT. For the asymmetric case, the RT and the NPT belong to the DP universality class, while for the symmetric case, they are related to the DI universality class.

The stochastic model we introduce is defined as follows. In the model, two different species of particles are deposited or evaporated on a one-dimensional substrate with periodic boundary condition. The two species are indicated by two colors (e.g., black and gray). The dynamics starts from a vacuum state, where no particle is in the system. A site is first selected at random, at which either deposition or evaporation of a particle is attempted with probability *p* (*p*/2 for black and $p/2$ for gray) and $1-p$, respectively. The deposition and evaporation are realized under the two conditions described below. First, a restricted solid-on-solid condition is imposed such that the height difference between nearest neighboring columns does not exceed 1. Second, the interaction between nearest neighboring particles within the same layer is considered, which is attractive (repulsive) between the same (different) species. When a particle with a certain color (e.g., black) arrives for deposition on a hollow between particles, the deposition is not allowed when both neighboring particles on each side are of the common species $(gray)$, but different from that of the newly arriving particle (black). Meanwhile, a particle with a certain color (e.g., black) is not allowed for evaporation when it is surrounded between the same species of particles (black). However, a particle can be deposited or evaporated whenever two neighboring particles on each side are of different species from one another, or one $~\rm (or~ both)$ of the neighboring sites is $~\rm (are)$ vacant. The dynamic rule is depicted schematically in Fig. 1. Since the dynamic rule is symmetric with respect to the particle species, each configuration has its own dual state that the occupied sites are identical, but one color is replaced by the other and vice versa, as shown in Fig. 1. When *p* is small, particles form small-sized islands which disappear after their short lifetime. Thus the interface is smooth. As *p* increases, depo-

FIG. 1. The dynamic rule for deposition (a) and for evaporation (b) for the symmetric case of the growth model. FIG. 2. (a) Double logarithmic plot (DLP) of $\rho_g(p,t)$ versus

sition increases and islands grow, until, above a critical value *pc* , islands merge and fill new layers completely, giving that the interface is unbounded from the bottom layer and becomes rough. Thus, the RT occurs at p_c , consistent with the critical point of the NPT. This stochastic model might be relevant to describe the surface growth by two-component particles such as the magnetic Eden model and the growth model with binary alloy $\lceil 15 \rceil$.

In an asymmetric version, one species (e.g., black) can distinguish itself from the other, whereas the gray species regards the black species as the same species. Then a gray particle cannot evaporate at the site where both neighboring particles are occupied by any species of particles, whereas a black particle can do whenever one of the neighbors is of a different species from its own one. Then the symmetry in the dynamic rule is broken, and the gray species flourish much more than the black. When all particles are of a single species, an extreme case of the asymmetric version, the model is reduced to the one by Alon *et al.* [2], where particles cannot evaporate at any site in terrace, and can do only at the edge of the terrace. The model defined so far is called the growth model hereafter to distinguish itself from the model below, called the monolayer model, confined in monolayer.

When the dynamics is restricted on monolayer, so that particle is not allowed to deposit on top of another particle, the model exhibits the NPT by varying the deposition probability p . In this case, a vacant (occupied) site corresponds to an active (inactive) site. Then there exist two inactive states, in each of which the entire system is filled with one single species of particles. As long as the symmetry is conserved, the two inactive states are equivalent and the monolayer version belongs to the DI universality class. For comparison, our monolayer model is similar to the generalized contact process proposed by Hinrichsen $|14|$, but the current model is much simpler because the model has one control parameter instead of two used in his model. Moreover, the model is easily generalizable to other cases including higher number of symmetric states or in higher dimensions.

We performed Monte Carlo simulations for both the growth model (the symmetric and the asymmetric cases) and the monolayer model by varying the deposition probability *p* and system sizes $L=10$ ~ 1000. Let us first discuss the numerical result of the growth model. We first measure the vacant site density $\rho_g(p,t)$, averaged over all runs, where the

time *t* for probabilities $p=0.4410$ (top), $0.4480(=p_c)$, and 0.4600 (bottom). The data are obtained for $L=100$, averaged over more than 500 configurations. The dashed and the dotted lines have slope 0.27 and 0.58, respectively, drawn for the eye. (b) DLP of $S(t)$ versus time *t* for the same cases as (a). (c) DLP of $\rho_g^{(s)}(p_c, t)$ versus *t* for different system sizes $L = 50$ (top), 100, 200, and 500. The dotted line has slope 0.58, drawn for the eye. Inset: DLP of τ_{φ} versus *L* at p_c . (d) DLP of $\rho_g^{(s)}(p, \infty)$ versus ϵ . The dashed line has slope 0.88, drawn for the eye. All plots (a) – (d) are for the symmetric case of the growth model.

subscript *g* means the growth model. $\rho_{\varrho}(p,t)$ saturates at finite value for $p < p_c$, and decreases to zero exponentially for $p > p_c$ in the long time limit as shown in Fig. 2(a). At criticality $p = p_c$, $\rho_g(p_c, t)$ scales algebraically as

$$
\rho_g(p_c, t) \sim t^{-\beta/\nu} \tag{1}
$$

For the asymmetric case, $p_c \approx 0.3796$ is estimated, and $\beta/\nu_{\parallel} \approx 0.16(1)$ is measured, in good agreement with the DP value, $\beta/\nu_{\parallel}(DP) \approx 0.1595$ [16,17].

For the symmetric case, it is found that $p_c \approx 0.4480$, which is much lower than the value of the monolayer model below. The exponent β/ν_{\parallel} is obtained to be $\approx 0.58(1)$, which is much deviated from the DI value, $\beta/\nu_{\parallel}(DI)$ $\approx 0.27 \sim 0.29$ [16]. These discrepancies may come from the suppression-effect by the particle on upper layer. For example, the particle A in Fig. 1 can evaporate in the monolayer version because one of neighboring particles are of the other color, however, it cannot evaporate in the growth version because of the existence of another particle on top of it. For comparison, for the asymmetric case, the particle A cannot evaporate even in the monolayer model, because of the existence of the two particles on each side regardless of their colors. Therefore, the suppression-effect appears strongly (weakly) for the symmetric (asymmetric) case. Since the evaporation process is suppressed, and $\rho_g(p_c, t)$ decays faster than the DI behavior as $\sim t^{-0.58}$. Note that the measured value ≈ 0.58 is twice as large as the DI value.

We consider the probability $S(t)$ that the system contains at least one vacant site on the bottom layer, and other sites are occupied by any species of particles. Note that $S(t)$ is different from the survival probability $P(t)$ conventionally used in the monolayer models $[16]$ in the sense that the probability $S(t)$ $[P(t)]$ counts the number of configurations that the bottom layer is filled with any species (a single species) of particles. As can be seen in Fig. $2(b)$, there exists a characteristic time τ_g such that for $t < \tau_g$, $S(t) = 1$, and for *t* $>\tau_g$, *S*(*t*) decays in the same way as ρ_g does. Thus the vacant site density $\rho_g^{(s)}(p_c,t)$, where the notation (s) means the average over the sample with at least one vacant site, decays as Eq. (1) up to τ_g , and is finite beyond τ_g as shown in Fig. 2(c). The steady state value $\rho_g^{(s)}(p_c, \infty)$ depends on system size *L* as $\rho_g^{(s)}(p_c, \infty) \sim L^{-\beta/\nu_{\perp}^{\circ}}$. We obtained β/ν_{\perp} $\approx 0.95(1)$, which is almost twice as large as the DI value, \approx 0.5. However, the dynamic exponent $z = \nu_{\parallel}/\nu_{\perp}$, which is defined via the characteristic time as $\tau_g \sim L^{\nu} \psi_{\perp}$, is measured to be $\nu_{\parallel}/\nu_{\perp} \approx 1.64(2)$. This numerical value is close to the DI value \approx 1.66 \sim 1.75 [16]. On the other hand, for ϵ = (p_c $-p$) > 0 , the steady state value may be written as $\rho_g^{(s)}(p, \infty)$ ~ ϵ^β . As shown in Fig. 2(d), the data do not fit well to a straight line for small ϵ , but are likely to approach a line asymptotically with slope $\beta \approx 0.88$, the DI value, for large ϵ , being far from p_c .

In the rough phase, the surface grows with finite velocity, which depends on the deposition probability as $v \sim (p \cdot p)$ $(-p_c)^y$. The velocity might be related to the inverse of the characteristic time τ_g via $v \sim a/\tau_g$, where *a* is lattice constant. If τ_g is written as $\tau_g \sim (p - p_c)^{-\nu}$ for $p > p_c$, followed by the scaling theory [16], the velocity exponent *y* would be equal to ν_{\parallel} . This relation is confirmed for the asymmetric case; the measured value $y \approx 1.67(8)$ is close to the DP value ν _|(DP) \approx 1.73. However, for the symmetric case, the measured value $y \approx 1.25(3)$ is much deviated from $\nu_{\parallel}(DI)$ \approx 3.17 \sim 3.25 [13], suggesting that the scaling behavior does not hold in the rough phase. This discrepancy may result from the suppression effect, which appears much strongly in the rough phase.

Next, we consider the surface fluctuation width in the rough phase, $W^2(L,t) = (1/L)\sum_i h_i^2(t) - [(1/L)\sum_i h_i(t)]^2$, where $h_i(t)$ denotes the height at site *i* at time *t*. The interface width behaves as

$$
W^{2}(L,t) \sim \begin{cases} t^{2\zeta/\zeta} & \text{for } t \ll L^{z}, \\ (-\epsilon)^{\chi}L^{2\zeta} & \text{for } t \gg L^{z}, \end{cases} \tag{2}
$$

where ζ is the roughness exponent and χ is the exponent to describe the roughness as a function of the deposition probability *p*. The exponent χ is measured to be $\chi \approx 0.34(1)$ $\lceil \approx 0.89(4) \rceil$ for the symmetric (asymmetric) case as shown in Fig. 3(b). The asymmetric value is close to $\chi \approx 0.92$ obtained from the single-species model $[2]$. The roughness exponent $\zeta \approx 0.50(1)$ is close to the one in the Edwards-Wilkinson (EW) universality class [18] and the Kardar-Parisi-Zhang (KPZ) universality class $|19|$ in one dimension, which is also confirmed via the height-height correlation function, $C^2(r) = \langle [h(r) - h(0)]^2 \rangle$, which behaves as a function of the distance *r* as $C^2(r) \sim r^{2\zeta}$ [Fig. 3(c)]. The numerical value of the growth exponent ζ/z varies between 1/4 and 1/3, depending on the deposition probability *p*. Since the growth velocity for $p > p_c$ is nonzero, the interface growth belongs to the KPZ universality class. At p_c , the roughness of surface exhibits the marginal behavior, $W^2 \sim \log t$ for *t* $\ll L^{z}$ and $W^{2} \sim \log L$ for $t \gg L^{z}$.

FIG. 3. (a) Plot of the velocity *v* versus $-\epsilon$. The dashed line $v=0.95*(-\epsilon)^{1.25}$ was obtained by a least-square fit. (b) DLP of W^2 versus $-\epsilon$ to measure the exponent x. The dotted line, a guideline to the eye, has slope 0.34 . (c) DLP of the height-height correlation function versus distance *r* at $p=0.9$. The data are well fit to a straight line with slope $2\zeta=1$. (d) DLP of W^2 versus *t* at probabilities $p=0.5$ and 0.9 (top). The dotted and dashed lines have slopes 0.49 and 0.62 (top) to guide to the eye. All plots (a) – (d) are for the symmetric case of the growth model with $L = 500$, and the data are averaged over 500 configurations.

Next, we discuss the numerical result for the monolayer model. The simulations were performed with two different initial configurations. For one case, every site is occupied by a single species of particle except one vacant site at $t=0$. Then the dynamics begins at the vacant site or its vicinity. This initial configuration is used in the defect dynamics $[16]$. The active site density increases with increasing time. We measure the survival probability $P(t)$ (the probability that the system is still active at time *t*), the density of the active site $\rho_m(t)$ averaged over all runs, where the subscript *m* means the monolayer model, and the mean-square distance of spreading of the active region $R^2(t)$ averaged over surviving runs. At criticality, $\bar{p}_c \approx 0.7485$, these quantities scale algebraically as a function of time as $P(t) \sim t^{-\overline{\delta}}$, $\rho_m(t) \sim t^{\overline{\eta}}$, and $R^2(t) \sim t^{2/\overline{z}}$, where the bar means the exponents of the monolayer model. It is measured that $\overline{\delta} \approx 0.28(1)$, $\overline{\eta} \approx 0.00$, and their sum $\overline{\delta} + \overline{\eta} = \overline{\beta/\nu_{\parallel}}$ is consistent with the DI value. The measured dynamic exponent $\overline{z} \approx 1.75(1)$ is also consistent with the DI value. For the second case, every site is vacant at $t=0$, which is the same initial condition as used in the growth model. In this case, the active site density decreases with increasing time as $\rho'_m(t) \sim t^{-\bar{\eta}t}$, where the prime means the exponents are from the second initial condition. The exponent $\overline{\eta}' \approx 0.27(1)$ is obtained. The survival probability behaves as $P'(t) \sim t^{-\delta'}$, and the exponent δ' ≈ 0.00 is obtained. Even though the two different initial configurations produce the different values of the exponents, their sums are close to each other, $\overline{\delta} + \overline{\eta} \approx \overline{\delta}' + \overline{\eta}'$, which is equal to β/ν_{\parallel} .

In summary, we have introduced an interface model with a twofold symmetry, exhibiting the RT and the NPT at the bottom layer, to show that the symmetry in the dynamics plays the role of classifying the universality class for the RT. Performing numerical simulations, it was shown that when the twofold symmetry is broken, the RT and the NPT belong to the DP universality class. When the symmetry is conserved, the dynamics at the bottom layer is affected by the particle on upper layer (the suppression effect), leading to that the critical point is considerably lowered and the vacant site density decays faster than the DI behavior with the exponent almost twice as large as the DI value. Nevertheless, the dynamic exponent of the model is close to the DI value, leading to the conclusion that the NPT is related to the DI universality class for the symmetric case. Finally, the behav-

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ior of the interface growth velocity in the rough phase cannot

Note added. Recently we learned of a similar work by Hinrichsen and Odor [20], motivated by the current work, on the roughening transition related to the DI universality class. However, their stochastic model is different from ours.

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