Growth in a restricted-curvature model

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The surface structure of a restricted-curvature model is studied. If evaporation and deposition are allowed equally, the surface width W increases as t^β with $\beta = 0.365 \pm 0.01$ $(d = 1 + 1)$ and $\beta = 0.24 \pm 0.01$ $(d = 2 + 1)$ being consistent with the results of a fourth-order linear equation which describes growth under surface diffusion. In the nonequilibrium situation, the average velocity of the surface height decreases exponentially with time and the surface becomes frozen in the long-time limit. Near this nonequilibrium pinning transition, the crossover length diverges as a power law in the deviation from equilibrium.

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There have been considerable recent efforts in studying the surface structure of various growth models [1]. Among them, the solid-on-solid (SOS) model has been extensively used [1–10] to study both equilibrium and nonequilibrium surface properties. The SOS model can be considerably simplified by restricting the height difference between the nearest neighbors without losing any generality. In this restricted solid-on-solid (RSOS) model, overhangs, and vacancies are not allowed and also the short wavelength fluctuations are suppressed. Specifically, nonequilibrium growth in the RSOS model [2] is well-described by the Kardar-Parisi-Zhang (KPZ) equation [11]. In fact, the RSOS model has led to some of the best numerical estimates of KPZ growth exponents. Here, we introduce a *restricted-curvature* (RC) growth model which has a restriction on the local surface curvature. We find that the RC model has a universality class different from the KPZ universality and, in addition, the nonequilibrium RC model leads to a new type of restricted-curvature-driven surface pinning transition where the long-time surface configuration becomes frozen and no further growth is allowed.

Most theoretical efforts concentrate on studying the surface structure of the growth models, especially on determining the dynamical critical exponents governing the surface fluctuations. The basic 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 [3]

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

where the scaling function $f(x)$ is x^β (with $\beta = \alpha/z$) for $x \ll 1$ and is constant for $x \gg 1$. The universality class of a growth model is determined by the values of the dynamical exponents α and β (or z). One of the major recent issues in the literature has been the universality class of various atomistic growth process, e.g., molecular beam epitaxy (MBE). It has been suggested [5-10] that some simple atomistic models for MBE growth may belong to a universality class different from KPZ class. While there is some recent experimental evidence [12] supporting this claim, the issue is still quite controversial. It would, therefore, be helpful if one could construct simple alternate models that would belong to the same universality class as these so-called "MBE growth models" whose distinguishing feature is that growth occurs under surface diffusion conditions, in that the deposited atoms relax (before incorporation into the growing film) by diffusing to the local kink sites (or, equivalently by maximizing the local coordination number). The important result of this paper is the introduction of an *equilibrium model*, namely the equilibrium RC model, which belongs to the same universality class as the nonequilibrium linear "MBE growth model" studied in several recent publications [5–8,10,13].

The fourth-order continuum linear equation, i.e., the linear "MBE growth model," describing growth under surface diffusion is given by

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu \nabla^4 h(\mathbf{x},t) + \eta(\mathbf{x},t), \tag{2}$$

where $\eta(\mathbf{x},t)$ is an uncorrelated Gaussian noise. This equation can be solved exactly giving $\alpha = (5-d)/2$ and $z = 4$, i.e., $\beta = (5-d)/8$. Atomistic simulation [5–10] shows that random deposition on SOS growth models allowing diffusion to local kink sites produces dynamical growth exponents given by this linear fourth-order differential equation, and our simple RC model, in the equilibrium case, has exactly the same exponents.

The growth rule of the equilibrium RC model is to randomly select a site on a $(d-1)$-dimensional substrate and then take a random action between deposition or evaporation (within the SOS restriction) with equal probability, provided the restriction on the local curvature $|\nabla^2 h| \leq N$ is obeyed at both the selected site and the nearest-neighbor sites where N is a preassigned fixed positive integer. If this RC condition is not satisfied, the corresponding deposition or evaporation event is forbidden. (No relaxation or hopping of the deposited atom is allowed in the model.) Thus, the model is analogous to the RSOS model, except that the restriction is on the local curvature $\nabla^2 h$ rather than on the height difference. Most of our simulations are performed with $N = 2$ or 6 in $d = 1 + 1$ and $N = 4$ or 6 in $d = 2 + 1$, starting from a flat surface with periodic boundary conditions in the $d-1$ dimensions. The values of the exponents are found

to be independent of N as long as N is greater than or equal to $2(d-1)$. The time t corresponds to the number of Monte Carlo steps. We find that this equilibrium RC model gives $\alpha \approx (5-d)/2$ and $\beta \approx (5-d)/8$ within our numerical accuracy in $d = 1+1$ and $d = 2+1$, and thus belongs to the same universality class as Eq. (2).

Since there is a restriction only on the curvature, the height difference between the nearest neighbors can be arbitrarily large. For $1 \ll t \ll L^z$, the surface width increases as t^β and eventually saturates when the parallel correlation $t^{1/z}$ is of the order of the lateral system size L. In Fig. 1, we show some typical surface configurations in the saturated regime for $L = 40$, $d = 1+1$, and N=2. Even though the slope $|\nabla h|$ varies slowly due to the curvature restriction, the slope can be arbitrarily large in contrast to other models, e.g., the RSOS model where $|\nabla h|$ cannot become very large.

To determine β, the exponent governing the rate of growth of the interface width, we measure $W(t)$ as a function of time for the system size $L = 100\,000$ $(d = 1+1)$ and 500 $(d = 2+1)$. Through the relation $W(t) \sim t^\beta$ for early time $t \ll L^z$, we obtain

$$\beta = \begin{cases} 0.365 \pm 0.01, & d = 1+1, \quad N = 6 \\ 0.24 \pm 0.01, & d = 2+1, \quad N = 6. \end{cases} \tag{3}$$

In each case 50 independent runs are averaged to get good statistics. Since the data in Fig. 2 are slightly curving upwards, these β values are consistent with $\beta = (5-d)/8$. [In $d = 1+1$, if we extrapolate to estimate β for $t \to \infty$, assuming a constant correction to scaling of the form $W^2(t) \sim t^{2\beta} + C$ where C is a constant, we get $\beta \approx 0.375$.]

To determine the roughness exponent α describing the saturation of the interface fluctuation, we use the relation $W(L) \sim L^\alpha$ for the system size L in the steady-state regime $t \gg L^z$. Since the value of z is around 4, it takes a very long time to arrive at the saturated regime. This has forced us to restrict our simulation system sizes to $L =$ 10, 20, 40, and 80 in d =1+1, and $L = 5$, 10, 20, and 40 in d =2+1. As shown in the inset of Fig. 2, from the log-log plot of $W(L)$ and size L, we get

$$\alpha = \begin{cases} 1.45 \pm 0.1, & d = 1+1 \\ 0.97 \pm 0.1, & d = 2+1. \end{cases} \tag{4}$$

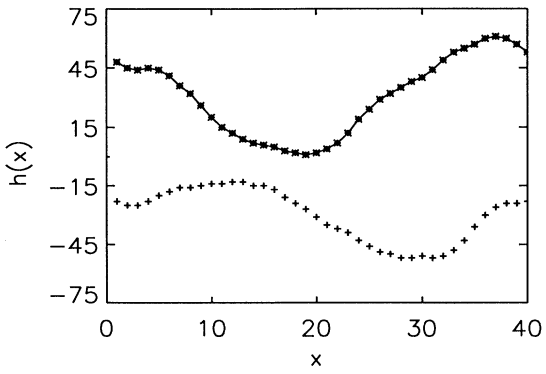

FIG. 1. Two typical surface configurations for the equilibrium RC model in the saturated regime for $t = 10\,000$ (upper curve: a constant 50 is added to h for clarity) and 20 000 (lower data) with $L = 40$, $N = 2$, and $d = 1+1$.

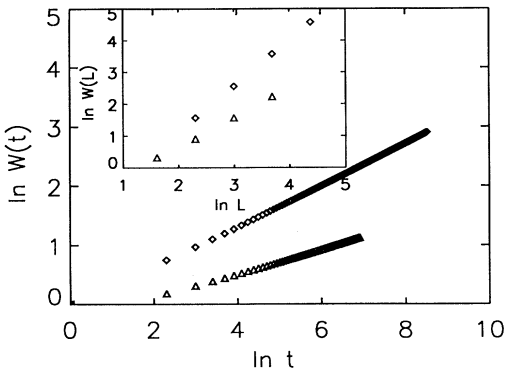

FIG. 2. Interface width $W(t)$ vs time on a logarithmic scale for $d = 1+1$ (diamond) and $d = 2+1$ (triangle) for the equilibrium RC model. Inset: interface width $W(L)$ in the saturated regime vs system size on a logarithmic scale for $d = 1+1$ (diamond) and $d = 2+1$ (triangle) with $N = 6$.

These values are consistent with $\alpha = (5-d)/2$ within the error bar. Since the values of β and α agree with the dynamical exponents of Eq. (2), we believe that the equilibrium RC model does indeed belong to the same universality class as Eq. (2).

The continuum Hamiltonian for the equilibrium RC model can be written as

$$H \sim \int d^{d-1}x \left| \frac{\nabla^2 h}{N} \right|^{2n}, \tag{5}$$

with n being a large number under the most general RC conditions. The corresponding Langevin dynamical equation [7], $\frac{\partial h}{\partial t} = -\frac{\delta H}{\delta h} + \eta$, becomes the same as the fourth-order linear equation given in Eq. (2) with $n = 1$. Thus, the Hamiltonian describing the equilibrium RC model is given by $H \sim \int d^{d-1}x |\frac{\nabla^2 h}{N}|^2$. (This is formally similar to the equilibrium RSOS model [2] or single step model [14] which is well described by the continuum Hamiltonian $H \sim \int \mathrm{d}^{\mathrm{d}-1}\mathrm{x} |\frac{\nabla h}{N}|^2$, leading to the Edwards-Wilkinson growth equation [15] $\frac{\partial h}{\partial t} = \nu_1 \nabla^2 h + \eta$.) Note that any curvature-dependent Hamiltonian, containing the leading term $|\nabla^2 h|^2$ in the functional, will have equilibrium fluctuations governed by Eq. (2) in the asymptotic sense. In fact, it is easy to show that the equilibrium fluctuations of such a Hamiltonian will have $\alpha = (5-d)/2$ by considering a random walk in $(d-1)$-dimensional curvature space.

In the equilibrium model, the trial probability of deposition P_+ is the same as the trial probability of evaporation $P_- = 1 - P_+$. If P_+ is greater than P_-, we have the nonequilibrium RC model with the average surface growing with time. For $P_+ = 1$, we find the average growth velocity $V = \langle \frac{\partial h}{\partial t} \rangle$ of the surface height to decay exponentially with time, becoming zero at long times when adding a particle at any site breaks the RC condition. In the nonequilibrium RC model the surface, therefore, becomes frozen at long times because no particle is allowed to stick at any site due to curvature restriction. This is the RC-driven pinning transition mentioned in the Introduction. Even for a small $\Delta P = P_+ - P_-$, the

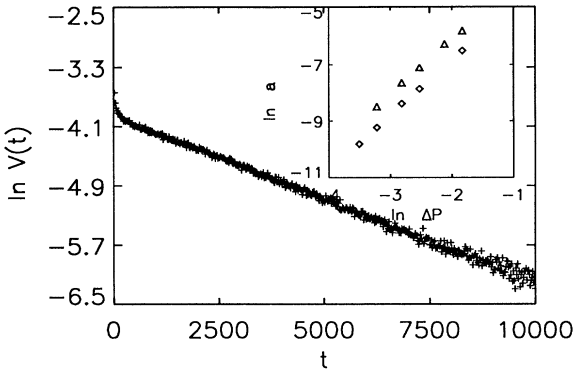

FIG. 3. $\ln V(t)$ vs time for nonequilibrium RC model with $\Delta P = 0.06$, $N = 2$ in d =1+1. The slope gives the negative decay coefficient $-a$, where $V(t) \sim e^{-at}$. Inset: $\ln a$ vs $\ln \Delta P$ for the nonequilibrium RC model in $d = 1+1$ (diamond) and $d = 2+1$ (triangle). The crossover length $t^* = 1/a$ diverges as ΔP approaches zero.

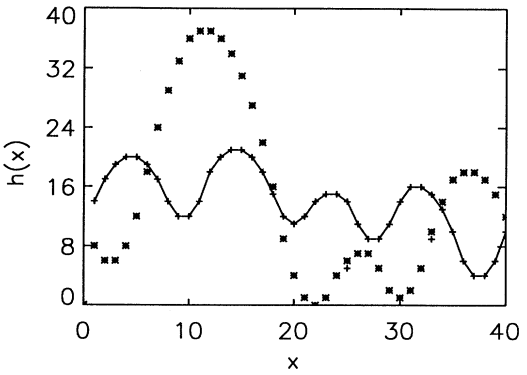

FIG. 4. Two frozen surface configurations for $\Delta P = 1$ (connected curve) and $\Delta P = 0.8$ (unconnected data) with $L = 40$, $N = 2$, and $d = 1+1$ for the nonequilibrium RC model.

velocity decreases exponentially $V(t) \sim e^{-at}$ where the decay coefficient a depends on ΔP. As an example, we plot $\ln V(t)$ against time in Fig. 3, getting a very good straight line plot for $\Delta P = 0.06$ and $N = 2$ in d =1+1. For very small ΔP, it takes a very long time for the RC condition to be operative, but we have verified that down to $\Delta P = 0.04$ ($d = 2+1$) and 0.03 ($d = 1+1$) the velocity decays exponentially. We postulate that this exponential decay of V happens for any nonzero ΔP. As shown in the inset of Fig. 3, the decay coefficient a seems to follow the power-law behavior $(\Delta P)^\delta$ with $\delta = 2.0 \pm 0.2$ (d=1+1) and $\delta = 1.96 \pm 0.2$ (d =2+1), supporting the conjecture that the transition happens at $\Delta P = 0$. If we define a crossover time $t^* \equiv 1/a$, then t^* diverges as $(\Delta P)^{-\delta}$ with $\delta \approx 2$. We emphasize that this depinning transition at $\Delta P = 0$ does not arise simply from a pinning potential but is driven by the RC condition. (For example, no such transition occurs in the RSOS growth model.) Since the surface becomes frozen [in the sense that $V(t)$ decays to zero] in the nonequilibrium RC model, we conclude that $\alpha = 0$. The exponents β and z are not well defined in the nonequilibrium RC model. In Fig. 4 we show some frozen configurations in the nonequilibrium RC model with vanishing growth velocity.

We do not yet have a theoretical understanding of the dynamical pinning transition in the nonequilibrium RC model. In analogy with the KPZ equation (which adds the second order nonlinearity $|\nabla h|^2$ to the $\nabla^2 h$ relaxation term of the Edwards-Wilkinson equation), we may consider a nonlinear equation of the form

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu \nabla^4 h(\mathbf{x},t) + \lambda [\nabla^2 h(\mathbf{x},t)]^2 - y_0 \sin[2\pi h(\mathbf{x},t)] + \eta(\mathbf{x},t) \quad (6)$$

as the generalization of Eq. (2) to describe the nonequilibrium RC model. The second term in the right-hand side is the nonlinearity arising from the curvature restriction [16]. The third term is due to the lattice structure preferring integer multiples of h. Since the deposition on the high curvature regime is not allowed, the λ term should be negative for $\Delta P \neq 0$. (There is a similar trend in the RSOS growth model [17].) For $y_0 = 0$, the nonlinear equation given by Eq. (6) has recently been numerically integrated [18] with the result $\alpha \approx 1.4$ in $d = 1+1$ without any frozen states [19]. In our nonequilibrium RC model $y_0 \neq 0$; we speculate that y_0 is a relevant parameter (in the renormalization-group sense) for nonzero λ. Unfortunately, we are unable to calculate analytically [20] the dynamical critical exponents of Eq. (6).

In conclusion, we have introduced a simple RC growth model which in the equilibrium case is in the same universality class as the recently studied [5, 6] linear "MBE growth equation" given by Eq. (2). In the nonequilibrium case, the model exhibits a novel pinning transition where the interface configuration becomes frozen at long times. The crossover to the depinning point is found to diverge as a power law in the deviation from equilibrium. We speculate on the possible continuum nonequilibrium nonlinear equation which may describe the RC growth model.

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[20] A single-loop dynamical renormalization-group treatment of Eq. (6) with $y_0 = 0$ does not lead to any nontrivial stable fixed point for $d \leq 4$, and there is no simple hyperscaling relation between the exponents α and z.