Kinetic Growth with Surface Diffusion: The Scaling Aspect

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We present computer simulations of kinetic growth models with a physically realistic surface diffusion process and without desorption. The results demonstrate that the asymptotic statistical scaling properties of the surface generated under these conditions are still correctly depicted by the Kardar-Parisi-Zhang (KPZ) theory. We show that surface diffusion nevertheless introduces a novel type of scaling at early times which will eventually cross over to the KPZ scaling. Furthermore, we make a clear connection between kinetic growth models and molecular-beam-epitaxy processes by illustrating the impact of surface diffusion on reducing the concentration of bulk defects.

Kinetic roughening in nonequilibrium surface growth has been a primary focus of research interest over the past few years. A novel feature of this phenomenon is the existence of scaling [1], i.e., if we start at $t=0$ from a flat surface of length L, we have

$$\xi_L^2(t) = \frac{1}{L^{d-1}} \sum_{\mathbf{r}} [h(\mathbf{r},t) - h_0(t)]^2 = L^{2\alpha} f(t/L^z), \quad (1)$$

where $\xi_L(t)$ is the rms roughness of the surface (also called the "surface width"), $h(\mathbf{r},t)$ is the height of the surface at position $\mathbf{r}$ and time t, $h_0(t)$ is the average height at time t, and $d'=d-1$ is the substrate dimension in d-dimensional space. The roughness exponent α characterizes the self-affine fractal nature of the surface represented by the scaling $\xi \sim L^{\alpha}$, in the long-time limit. At the early stage of growth, $t \ll L^z$, the scaling function $f(t/L^z)$ is such that $\xi \sim t^{\beta}$, where $\beta = \alpha/z$ and z is the dynamic exponent. Simulations of various discrete growth models [1–4] have verified this scaling despite their different atomistic details. It is generally believed that the essential physics of this universality class is captured by the continuum theory of Kardar, Parisi, and Zhang (KPZ) [5] in which surface (interface) position $h(\mathbf{r},t)$ is assumed to be governed by the nonlinear equation

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta. \quad (2)$$

While desorption, and other surface relaxation processes, contribute to the first term on the right-hand side [6], the nonlinear term is attributed to the dependence of growth velocity on local surface orientation. $\eta(\mathbf{r},t)$ is an uncorrelated noise with Gaussian distribution and zero mean, which corresponds to the fluctuations in the incident flux. Theoretical analysis [5] of this equation and numerical simulations of relevant discrete models [1–3] indicate that for growth on a one-dimensional substrate ($d=1+1$), $\alpha = \frac{1}{2}$, $\beta = \frac{1}{3}$, and $z = \frac{3}{2}$. The values of the exponents are less definite due to theoretical difficulties and numerical constraints.

The self-affine fractal surfaces as represented by the scaling described above have been observed in numerous direct experimental measurements [7]. These measurements have provided firm support to the notion of the scaling as a valid and useful way to characterize real surfaces and the relevance of those simple theoretical models to low-temperature thin-film growth processes.

In an effort to study surface growth problems related to molecular-beam epitaxy (MBE) where surface diffusion, rather than desorption, is a dominating factor for surface morphology, a couple of groups [8,9] have investigated a simple (1+1)-dimensional solid-on-solid (SOS) growth model. In their model, particles are randomly added onto the top of columns of occupied sites and then are allowed to hop to the top of a nearby column with a kink site (within nearest l columns). They found that while the scaling ansatz (1) still holds, the growth exponents are given by, in 1+1 dimensions, $\alpha = 1.5$, $\beta = 0.375$, and $z = 4$. These results are consistent with the ones obtained from the analysis of a linear diffusion equation [6,10]

$$\frac{\partial h}{\partial t} = -\nu_1 \nabla^4 h + \eta. \quad (3)$$

However, as pointed out by Wolf and Villain [8], this coincidence is due to the large exponent α and the limited lattice size L used in the simulations. Including a lowest-order nonlinear term regarded as relevant to diffusion [8], Lai and Das Sarma [11] have proposed an alternative continuum equation to describe kinetic growth under "ideal" conditions of MBE (no desorption and bulk defects):

$$\frac{\partial h}{\partial t} = -\nu_1 \nabla^4 h + \lambda_1 \nabla^2 (\nabla h)^2 + \eta. \quad (4)$$

The growth exponents for this equation are given as $\alpha = 1$, $\beta = \frac{1}{3}$, and $z = 3$ in 1+1 dimensions.

It is puzzling to notice that the roughness exponent α obtained from Eq. (4) is larger than that in the KPZ case, which implies that with surface diffusion the surface would be, in principle, *rougher* than that in the case in which desorption is the only means of surface relaxation. This is also illustrated in the discrete model simulation of Wolf and Villain [8] in which the generated surface is ex-

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tremely rough with very high steps ("cliffs"). In addi-
tion, the SOS model used in these simulations yields an
unphysical roughness exponent $\alpha \geq 1$. A careful exam-
ination, however, reveals that the relaxation rule em-
ployed in this model [8,9] actually allows jumps between
neighboring columns for particles to reach a favored
bonding position (kink site) despite the high steps. This
is not a physical process because the cliff has also to be
considered as a part of the surface and particles can only
travel on it one step at a time.

In order to demonstrate the real effect of surface
diffusion on morphology and dynamic scaling, we have
carried out detailed simulations of a ballistic deposition
model and a random deposition SOS model, both with a
physical surface diffusion process. The results we present
in this Letter show that, except for an early time cross-
over, the scaling of the surface allowing for surface
diffusion is still given by that found in the KPZ equation.
Our results indicate that in the process of kinetic deposi-
tion and diffusion the terms $\nabla^2 h$ and $(\nabla h)^2$ are intrinsi-
cally built in and eventually determine the surface scaling
behavior. We will also point out that bulk defects (i.e.,
vacancies and overhangs) are physically present in the
process and should not be suppressed artificially as in the
SOS type of models. Rather, they will be annihilated as
the consequence of a *complete* surface diffusion process
as demonstrated in the (lattice-matched) MBE growth.

We start out with the ballistic deposition model, which
is argued to be relevant to vapor deposition processes
[12]. In the original model, particles following linear tra-
jectories are added randomly, one at a time, onto a grow-
ing surface and stick where they land. This growth rule
allows sticking of particles to the side of columns and
creation of voids and overhangs. No relaxation in the
surface is taking place. For the model we study here,
however, we have implemented a physically realistic pro-
cess for the just-deposited particle to diffuse. Immediate-
ly after the deposition, the particle moves via random
walk along the surface. It stops when it reaches either a
kink site (the site with two bonding neighbors in 1+1 di-
mensions) or a trapping site (with three bonding neigh-
bors), or when it has moved L_{RW} steps on the surface.
(A more detailed, but much more computationally inten-
sive diffusion model involving diffusion from kink sites
has also been simulated and shown to produce the same
statistical scaling properties. Details of the algorithm will
be presented elsewhere.) Note that a vertically exposed
region is also a part of the surface. The simulations are
performed in 1+1 dimensions with a varying number of
random walk steps L_{RW}.

In Fig. 1, we present plots of ξ^2 vs t for different L_{RW}.
The system size is $L = 2500$ and the result is averaged
over fifty samples. It clearly shows that in spite of a
different early-time scaling regime which we will discuss
later, the asymptotic scaling behavior for the ballistic
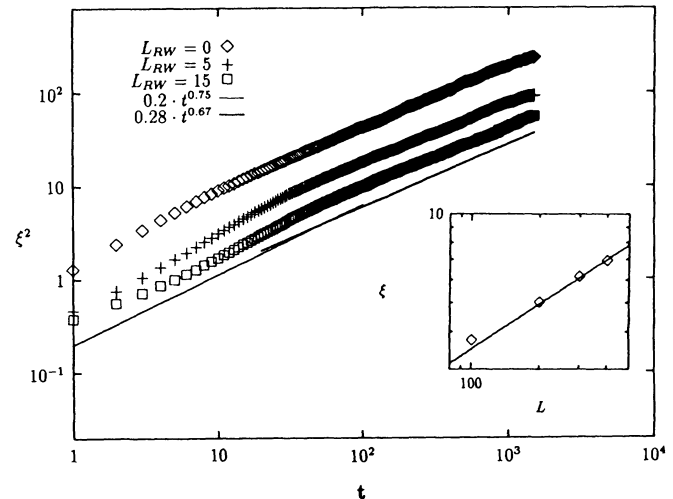deposition with diffusion is still $\xi \sim t^{1/3}$. However, it hap-

FIG. 1. ξ^2 vs t for the ballistic deposition model with
($L_{RW} = 5, 15$) or without ($L_{RW} = 0$) surface diffusion. The re-
sults are for $L = 2500$ (1+1)-dimensional systems, averaged
over fifty samples. Inset: The straight line corresponds to
$\xi = 0.35L^{1/2}$. The data points are for $L = 100$, 200, 300, and
400, respectively, and averaged over fifty samples.

pens that $\beta = \frac{1}{3}$ is true for both Eqs. (2) and (4) in 1+1
dimensions. In order to distinguish between these two
different types of scaling, we have measured the effective
roughness exponent α from the steady-state width of
smaller systems. The result in the inset of Fig. 1 shows
that for these systems α is $\frac{1}{2}$ which is the value for the
KPZ scaling, and differs from the value of unity predict-
ed for the Lai-Das Sarma scaling. Hence, this indicates
that the asymptotic scaling for the ballistic deposition
model with surface diffusion is dictated by the KPZ
theory.

In fact, this result is fairly straightforward to com-
prehend. As illustrated before [2,13], the ballistic deposi-
tion model contains the ingredients that make up the
KPZ equation (2). The inclusion of the surface diffusion
mechanism only adds additional terms, such as $\nabla^4 h$, to
Eq. (2). A power counting analysis [5] can be used to
show that the higher-order terms beyond those in Eq. (2)
are irrelevant in the renormalization process, and there-
fore the asymptotic scaling is always determined by the
KPZ equation.

On the other hand, the random deposition SOS model
[1] does not allow for intercolumn interactions. The
model can be described by $\partial h/\partial t = \eta$ and the surface
width ξ always scales with $t^{1/2}$. In an SOS model, voids
and overhangs in the bulk are suppressed. We have car-
ried out simulations of the random deposition SOS model
incorporating the same random-walk surface diffusion
process described above. Note that the model we study
here is different from a previously studied "random depo-
sition model with surface diffusion" [14] which discusses

height "diffusion" rather than capillarity-driven surface diffusion [15] concerned here.

The results of the simulations are plotted in Fig. 2. As a reference, the scaling for the original random deposition model is also shown. We can see that with just one diffusion step allowed ($L_{RW}=1$), the scaling changes dramatically from $\xi \sim t^{1/2}$ to an asymptotical form $\xi \sim t^{1/3}$, which is independent of L_{RW}. Notice that the surface width (roughness) decreases with the increase of L_{RW}. The measured exponent $\alpha \sim \frac{1}{2}$ as shown in the inset indicates that once again the KPZ type of scaling prevails. This implies that kinetic surface growth with diffusion is not only described by terms like $\nabla^4 h$ (and relevant nonlinear terms) as previously known [15], but is also determined by the dynamics coupled with local surface structures as depicted by the KPZ equation. Eventually, the KPZ scaling dominates.

Let us now examine the early-time scaling regime and the crossover from this regime to the KPZ scaling regime. In both Figs. 1 and 2, there is evidence for a true scaling regime before the crossover, which is different from the transient seen in the original models ($L_{RW}=0$). A fit to the data of the ballistic deposition model with $L_{RW}=5$, 10, and 15 gives $\beta=0.45$, 0.42, and 0.40, respectively. These values are close to, but larger than $\beta=0.375$, valid for the models described by Eq. (3) [8,9]. It is possible that β may approach the asymptotic value $\beta=0.375$. Though this conjecture remains to be verified, it is conceivable that the scaling of Eq. (3) may set in at a smaller length scale before the growth rate becomes heavily dependent on the surface orientation demarcating the
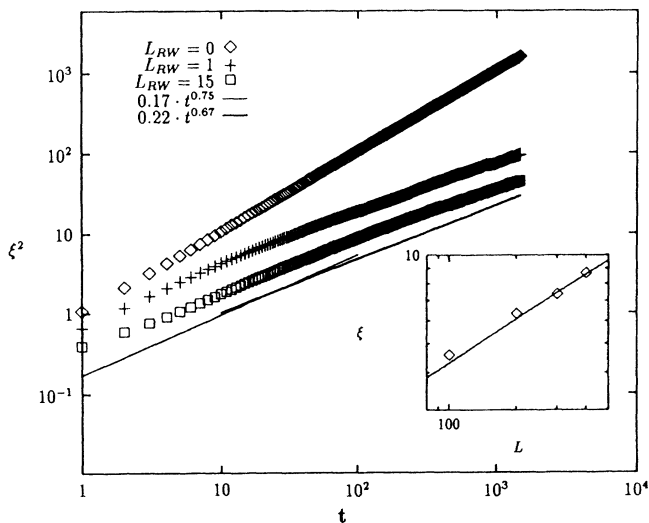
point at which the KPZ scaling takes over. It is also interesting to observe that the onset of the crossover shifts to a later time with larger L_{RW}. This is due to the fact that the contribution from $\nabla^4 h$ term to the growth process (as reflected in its coefficient v_1) is greater with larger L_{RW}.

In an effort to investigate the impact of surface diffusion on bulk defects and to make a connection between the models studied here and growth processes such as MBE, we have measured the bulk density ρ (far below the surface) as a function of L_{RW}. In Fig. 3, we plot ρ vs L_{RW} for the ballistic deposition model and the random deposition SOS model. It shows that as the number of diffusion steps L_{RW} increases, the density increases, approaching the ideal lattice density $\rho=1$. Moreover, we observe that for large L_{RW}, we have

$$1-\rho \sim 1/L_{RW}^{1.25},\qquad(5)$$

as shown in the inset of Fig. 3. This is also verified by the measurement of growth velocity v. Note that $v \sim 1/\rho$, thus we should have $v-1 \sim 1/L_{RW}^{1.25}$. On the other hand, an SOS model would generate a perfect bulk structure with $\rho=1$. However, as illustrated in Fig. 3, once surface diffusion is implemented in the model, vacancies are created in the bulk as the bulk density ρ drops from 1 for $L_{RW}=1$. Then with the increase of L_{RW}, the number of defects decreases and ρ approaches unity again. The results presented above clearly demonstrate that with enough surface diffusion steps we should be able to achieve a better bulk structure and a smoother surface, as in the case of molecular-beam epitaxy.

In summary, we have carried out simulations of surface growth models that incorporate realistic surface diffusion and deposition without desorption. Our results have shown that the asymptotic statistical scaling properties of
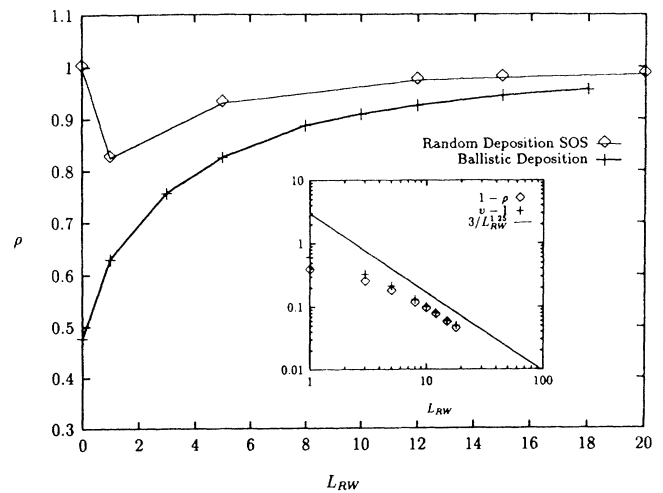

FIG. 2. ξ^2 vs t for the random deposition SOS model with ($L_{RW}=1,15$) or without ($L_{RW}=0$) surface diffusion. The results are for $L=2500$ $(1+1)$-dimensional systems, averaged over fifty samples. Inset: The straight line corresponds to $\xi=0.43L^{1/2}$. The data points are for $L=100$, 200, 300, and 400, respectively, and averaged over fifty samples.

FIG. 3. Plots of bulk density ρ vs number of diffusion steps L_{RW}. Inset: The curves, $1-\rho$ vs L_{RW} and $v-1$ vs L_{RW}, are for the ballistic deposition model with surface diffusion.

the surface generated under these conditions are still correctly described by the KPZ theory. This conclusion is consistent with that of a recent report by Kessler, Levine, and Sander [16] in which surface diffusion has been included in a different manner into the ballistic deposition model. Our results have also demonstrated that surface diffusion nonetheless introduces a novel early-time scaling regime which will eventually cross over to the KPZ scaling. Moreover, we have made a plausible connection between kinetic growth models and MBE processes by illustrating the impact of surface diffusion on reducing the concentration of bulk defects. Further studies are needed to understand the early-time scaling regime and to extend the model to realistic 2+1 dimensions.

Note added.— Most recently, Siegert and Plischke [17] proposed a model to study the instability in surface growth with diffusion. Their model is still of SOS nature and yields a roughness exponent $\alpha > 1$. However, combining the model in this Letter with part of the model of Siegert and Plischke, a surface diffusion model, in which random walks by the diffusing particles on the surface (not random hopping from column to column) are driven by the energy difference between steps with a probability related to $\exp(-\beta\Delta E)$, will provide us with valuable information about the temperature dependence of surface diffusion.

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