PHYSICAL REVIEW LETTERS

VOLUME 62 | 29 MAY 1989 | NUMBER 22

Anomalous Roughening in Growth Processes

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(Received 14 March 1989)

We study the roughening of a growing surface near a morphological transition within a general scaling framework. For a class of systems, where the transition can be related to directed percolation, the anomalous roughness at the critical point is at most logarithmical. In two-dimensional simulations we find $w^2 \sim \log L$, where w is the width of the surface and L is the substrate size.

PACS numbers: 05.40.+j, 05.90.+m, 61.50.Cj

What is the morphology of a growing surface? This nonequilibrium problem has attracted increasing interest during the last few years.[1] Even for the simple Eden-type growth which produces compact clusters different morphologies can be found characterized by different degrees of surface roughness. They can be distinguished by the roughness exponent ζ describing the algebraic dependence of the surface width w on the linear size L of the substrate on which the cluster grows: $w \sim L^{\zeta}$. Starting from a flat substrate the width increases with time t as a power law $w \sim t^{\zeta/z}$ for $t \ll L^z$. The general scaling behavior can be summarized in the form[2]

$$w = L^{\zeta} f(t/L^z)\,, \tag{1}$$

where $f(c) \sim c^{\zeta/z}$ for $c \ll 1$ and $f(c) \sim \text{const}$ for $c \gg 1$.

The understanding of the growth of rough surfaces was substantially improved by Kardar, Parisi, and Zhang[3] (KPZ), who first introduced the nonlinearity due to lateral growth into the Langevin equation[4] for the local height h of the surface above the substrate,

$$\partial_t h = \lambda[1 + \tfrac{1}{2}(\nabla h)^2] + \gamma \nabla^2 h + D\eta\,, \tag{2}$$

where λ is the normal growth velocity, γ an effective surface tension, and D the strength of the (white) noise η. Mapping Eq. (2) onto the Burgers equation the exact values of the exponents could be obtained in two dimensions ($\zeta = \frac{1}{2}$ and $z = \frac{3}{2}$). Furthermore, surface growth problems obeying (2) are related to polymer physics,[3] spin models,[5,6] as well as the dynamics of a sine-Gordon chain.[7] The nonlinearity guarantees the invariance of Eq. (2) with respect to infinitesimal tilting which is responsible[3] for the scaling relation[5,8]

$$\zeta + z = 2\,. \tag{3}$$

Based on a renormalization-group investigation of the KPZ equation it has been predicted[3] that for space dimensions $d > 3$ a morphological transition should occur between a weak coupling regime with the mean-field exponent[4] $\zeta = 0$ and a strong coupling region with nontrivial exponents $\zeta > 0$. Simulations[9] show a continuous dimensional dependence of the strong coupling exponents which obey the scaling relation (3) and support the expectation that they approach the mean-field values for $d \to \infty$.

Transitions from a smooth surface (with finite width, $\zeta = 0$) to a rough one (with diverging width, $\zeta > 0$) are well known from thermal systems. Equilibrium shapes of three-dimensional crystals provide examples for these roughening transitions. By analogy we shall call all morphological transitions between a smoothly growing surface and a rough one kinetic roughening transitions. Examples have been found besides the KPZ transition, in two-[10] and three-dimensional growth models.[11]

In this Letter we present a general scaling picture for morphological transitions between two phases of different roughness, and we shall apply it to a class of models where the connection with directed percolation allows us to make specific predictions about anomalous roughening. Suppose there is a transition at a critical value p_c of a parameter p between two morphologies $i=1,2$ characterized by the exponents ζ_i, z_i, and that close to the transition point a new diverging length $\xi \sim |\epsilon|^{-\nu}$ influences the roughness ($\epsilon = p - p_c$). Then we propose the following scaling form of the surface width:

$$w(\epsilon,L,t) \sim \xi^{\zeta'} f_i(L/\xi, t/\xi^{z'}) , \tag{4}$$

with the scaling function f_1 (f_z) above (below) the transition. Implicitly we assumed that ζ' as well as z' are the same for $\epsilon > 0$ and $\epsilon < 0$.

Sufficiently far from the transition, (4) must reproduce the normal scaling (1). It follows that

$$\lim_{a,b \to \infty} f_i(a,b) \sim a^{\zeta_i} g_i(b/a^{z_i}) ,$$

so that far from p_c

$$w(\epsilon,L,t) \sim \xi^{\zeta' - \zeta_i} L^{\zeta_i} g_i(\xi^{z_i - z'} t/L^{z_i}) \tag{5}$$

as in (1). Equation (4) describes the crossover between the two phases. Since the width remains finite for any fixed L and t, the divergent factor $\xi^{\zeta'}$ in (4) must be compensated by a suitable power-law behavior of $f_i(a,b)$ in the limit $a \to 0$ with $b/a^{z'}$ fixed. Therefore, at the critical point the surface shows roughening with anomalous exponents ζ', z':

$$w(0,L,t) \sim L^{\zeta'} g(t/L^{z'}) . \tag{6}$$

In a class of stochastic growth models the physics underlying the morphological transition is sufficiently well understood that the anomalous exponents can be predicted. These are models with a maximal velocity by which the uppermost point of the surface can propagate. Furthermore, the mass increase (growth rate) must be tunable independently. For small growth rate the surface propagates with a velocity smaller than the maximal one, so that it is expected to show normal roughness. If the growth rate is increased until the surface propagates with maximal velocity, it always feels the global constraint and cannot get rough anymore. Therefore, one has a morphological transition between phases with $\zeta_1 > 0$ and $\zeta_2 = 0$. The transition is triggered by directed percolation:[10] The stochastic growth process defines an effective local transition probability of reaching the level corresponding to the maximum velocity at every time step, i.e., an "occupation probability" for percolation through directed paths.

As an example, we consider the polynuclear growth (PNG) model[12] on the square lattice. The surface is described by a single-valued function $h(x,t)$; i.e., it consists of horizontal terraces and up and down steps. Growth proceeds in the y direction by repeating the following two processes in one time step: (i) *First* particles are deposited randomly on the surface ("nucleation"); i.e., the height $h(x,t)$ increases by 1 with probability p at every coordinate x. (ii) *Then* the terraces grow laterally; i.e., upward (downward) steps move deterministically towards the left (right) by u lattice constants until they vanish by collision.

In this model the maximum velocity is one lattice constant per time step. In the smooth phase a finite portion of the surface reaches the maximum height t at time t. This requires that the probability of nucleation on the uppermost terraces be higher than a (percolation) threshold k. At the transition the density of terraces at height t vanishes so that close to p_c one may consider an isolated terrace of size $2u+1$. The probability of a critical nucleation event is then $1-(1-p_c)^{2u+1}$, i.e., $p_c = 1-(1-k)^{1/(2u+1)}$ in excellent agreement with the simulation results (see Fig. 1).

The order parameter of the smooth phase is the same as in the corresponding directed percolation problem, namely, the density $\rho(\epsilon,L,t)$ of sites at the maximal height $h=t$,

$$\rho(\epsilon,L,t) = \xi_r^{-\beta/\nu_r} \phi(L/\xi_r, t/\xi_t) , \tag{7}$$

where $\xi_r \sim \epsilon^{-\nu_r}$ and $\xi_t \sim \epsilon^{-\nu_t}$ are the transversal and longitudinal correlation lengths known from the theory of directed percolation.[13] This implies that at $p = p_c$ the set of points which reach the level $h=t$ is getting fractal with the dimension $1-\beta/\nu_r$, and that ρ decays according to the power law

$$\rho \sim t^{-\beta/\nu_t} . \tag{8}$$

Comparing (7) and (4) it is natural to identify ξ_r and ξ_t with ξ and $\xi^{z'}$, respectively, so that

$$\nu = \nu_r, \quad z' = \nu_t/\nu_r . \tag{9}$$

The physical picture behind this identification is the following: The typical distance between the terraces at height t is equal to the transversal size ξ_r of the holes in the corresponding percolation cluster. Up to this length scale the surface develops anomalous roughness: $\omega \sim \xi_r^{\zeta'}$, which agrees with (5) ($\zeta_2 = 0$) if $\xi = \xi_r$. As it takes ξ_t

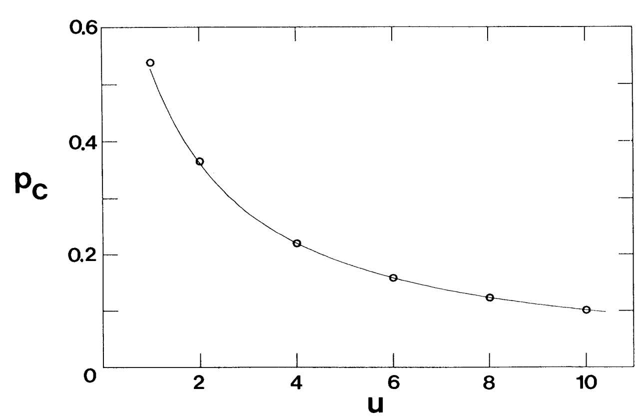

FIG. 1. Phase diagram $p_c(u)$ of the two-dimensional PNG model. Circles correspond to numerical results. The full curve is the fit $p_c = 1 - 0.1056^{1/(2u+1)}$.

until the distribution of the holes becomes stationary, it is clear that this is the characteristic time $\xi^{z'}$.

Let us now describe the transition from the smooth to the rough phase. It can be considered as a wetting transition if we regard the line $y=t$ as a wall, the space between the wall and the surface as filled by liquid, and that between the surface and the substrate as filled by vapor. Then complete wetting takes place for $p<p_c$. We define the velocity V of the thickening of the liquid layer as the order parameter of the rough phase,

$$V=1-v \quad \text{with} \quad v=\partial_t \bar{h}(t), \tag{10}$$

where $\bar{h}(t)$ is the average height. By analogy with (7) we make the scaling assumption

$$V(\epsilon,L,t)=\xi_r^{-\beta'/\nu_r}\psi(L/\xi_r,t/\xi_t). \tag{11}$$

Now we present an argument why β' should be equal to ν_t. This is the essential simplification which allows us to predict the exponent ζ'. In the stationary state for $p>p_c$ the surface moves with maximal velocity: $\bar{h}(t_0+t)=\bar{h}(t_0)+t$. However, for $p<p_c$ there exists a characteristic time τ after which the surface stays behind by one lattice constant compared to the position it would have reached with the maximal velocity: $\bar{h}(t_0+\tau)=\bar{h}(t_0)+\tau-1$. This is just the time for which directed percolation correlations survive, i.e., $\tau\sim\xi_t$. Hence, $V=1/\tau\sim\xi_r^{-\nu_t/\nu_r}$. Comparison with (11) shows that $\beta'=\nu_t$. As a consequence, one gets at p_c

$$V\sim 1/t. \tag{12}$$

Obviously, the surface has to fit into the interval between the average height and $y=t$, so that

$$w<\text{const}\times\int V\,dt\sim\log t. \tag{13}$$

Thus ζ'/z' and therefore ζ' have to be zero.

It is known[13] that for $p>p_c$ percolation is sustained within the angle $\arctan(\xi_r/\xi_t)$. It corresponds to a finite spreading velocity of surface perturbations. The characteristic relaxation time is therefore proportional to the substrate size L, i.e., $z_2=1$. Another consequence is that clusters grown from a seed have facets[10] which vanish at p_c like $\epsilon^{\nu_t-\nu_r}$ implying the same critical behavior of the cusp angle in the Wulff plot.[14]

In our simulations of the PNG model on the square lattice we first calculated the order parameter ρ which was used to locate the phase transition (Fig. 1). At p_c we observed power-law behavior according to (8) with $\beta/\nu_t\approx 0.16$ in full agreement with directed percolation theory[13] ($\beta=0.28$, $\nu_t=1.73$, and $\nu_r=1.10$ for $d=2$).

Far from the transition point, we obtained in the rough phase the universal exponents corresponding to a growth described by Eq. (2), i.e., $\zeta\approx\frac{1}{2}$ and $\zeta/z\approx\frac{1}{3}$. For the faceted phase we observed the cusp in the Wulff plot which we obtained by measuring the growth velocity over a tilted substrate.[14]

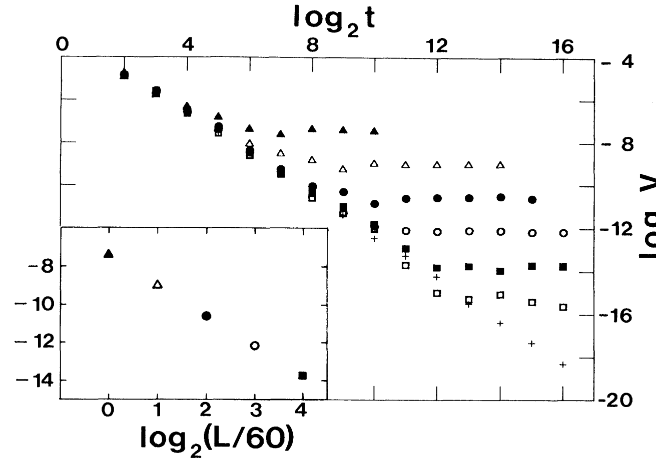

FIG. 2. Scaling of the order parameter V as a function of time t in the $d=2$ PNG model at $p_c=0.221$, $u=4$. Symbols are explained in Fig. 3. Inset: Stationary values of V as a function of substrate size L.

Detailed calculations for the anomalous roughening were carried out for $u=1$ ($p_c=0.539\pm0.001$) and $u=4$ ($p_c=0.221\pm0.001$). Typically 200 runs were taken with $L=60\times 2^n$, $n=0$–5, 8, and the time went up to $t=2^{16}$. Figure 2 shows the numerical verification of (12). The slope on a $\log V$ vs $\log t$ plot for p_c is -1.0 ± 0.1. Based on Eq. (11) one expects $V(L,t\to\infty)\sim L^{-z'}$. From the inset in Fig. 2 we obtain $z'=1.58\pm0.05$ in accordance with percolation theory. The square of the surface width was found to increase logarithmically in agreement with (13) and has logarithmic size dependence (cf. Fig. 3):

$$w^2\sim\log t, \quad w^2\sim\log L. \tag{14}$$

In summary we have presented a general scaling pic-

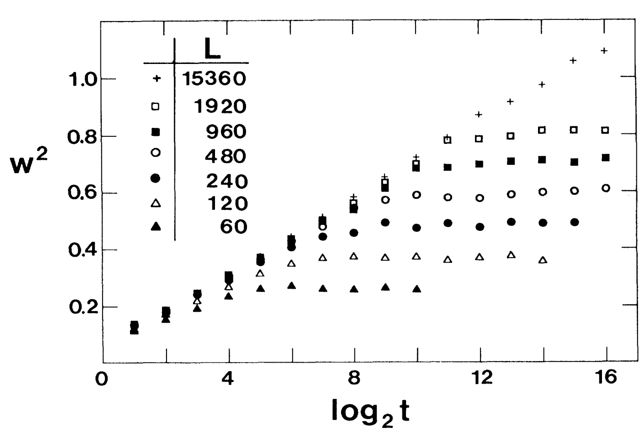

FIG. 3. Anomalous roughening in the $d=2$ PNG model ($p_c=0.221$, $u=4$). w is the surface width, t the time, and L the substrate size.

ture of anomalous roughening close to transitions in the morphology of growing rough surfaces. In a class of models with kinetic roughening the relation to directed percolation leads to the solution $z' = \nu_t/\nu_r$ and $\zeta' = 0$. This is a general result which applies to all models with the described roughening mechanism in any dimension. In particular this implies that above the upper critical dimension for directed percolation, $d \geq 5$, one obtains the mean-field value $z' = 2$. The anomalous exponents do not obey the scaling relation (3) because the invariance with respect to infinitesimal tilting of the growth direction is violated. Our numerical results for two dimensions are in full agreement with the theory. One cannot exclude that for $d > 3$ this transition interferes with the transition between the strong and weak coupling regions related to Eq. (2). The investigation of this question, and the determination of the anomalous roughening for the KPZ and other morphological transitions remain interesting future tasks.

We benefitted from valuable remarks by J. Krug and a discussion with T. Nattermann. This work was performed within Sonderforschungsbereich (SFB) 341 of the Deutsche Forschungsgemeinschaft (DFG). J. K. thanks the Humboldt Foundation for support.

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