Surface Roughening in a Hypercube-Stacking Model

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We study in $d+1$ dimensions a new deposition and evaporation model of a d-dimensional surface which bears a Potts-spin representation. For the pure deposition case, our simulations on systems up to $11\,520^2$ sites in $d=2$ and 2×192^3 sites in $d=3$ yield roughness exponents which violate recent conjectures. Including evaporation, we observe a nonequilibrium surface-roughening transition in $d=3$, but only a smooth crossover behavior in $d=2$. A logarithmic anomalous scaling form for surface width at the transition is conjectured.

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Surface roughening due to thermal fluctuations has been studied extensively over the years.[1] There now exist well-established theories[1,2] as well as exactly solvable models[1,3] which come to fair agreement with observed surface roughening in copper[2] and other experimental systems. In certain class of growth processes, such as Eden growth[4] and vapor deposition,[5] the moving surface of a *compact* cluster may also become rough under a stochastic growth rule. The scaling properties of the surface height fluctuation and characteristics of possible nonequilibrium roughening transitions have been the topic of a number of recent numerical and analytical investigations.[6-17]

Kardar, Parisi, and Zhang proposed a nonlinear Langevin equation

$$\partial h/\partial t = \nu\nabla^2 h + (\lambda/2)(\nabla h)^2 + \eta(\mathbf{x},t)\,, \tag{1}$$

for the local growth of the profile $h(\mathbf{x},t)$ of a moving interface above a d-dimensional flat substrate.[13] The first two terms on the right-hand side of (1) describe surface relaxation and a correction to the growth velocity due to a local tilt of the surface, respectively. The third term is a random variable which for our purpose will be assumed to be a white noise of variance D. Simple scaling arguments (power counting) as well as a one-loop renormalization-group (RG) calculation applied to (1) show that weak noise ($D\lambda^2/\nu^3 \ll 1$) is relevant for $d<d_c=2$, and irrelevant for $d>d_c$.[13] The RG analysis indicated the possibility of a nonequilibrium roughening transition from the weak-coupling to a strong-coupling regime ($D\lambda^2/\nu^3 \to \infty$) for $d>d_c$. It has also been suggested that anomalous roughening behavior may arise at the transition.[17]

Numerical simulations of Eden growth[6,7] and ballistic deposition[8-10] models show that the mean-square width of a surface grown from a flat substrate of linear size L at $t=0$ can be put in the scaling form[18]

$$w^2(t) \approx L^{2\zeta} F(t/L^z)\,, \tag{2}$$

where $F(x)\sim x^{2\beta}$ ($\beta\equiv\zeta/z$) for $x\ll1$ but becomes constant for $x\gg1$. Analysis of Eq. (1) provided the basis for the scaling and universality of roughness exponents among various growth models.[13,14] In particular, it was shown[8,13,19] that ζ and z satisfy the scaling law $\zeta+z=2$, in good agreement with numerical findings. However, the precise values of ζ and β are known only in $d=1$, where there exist exactly soluble models,[20] as well as other analytical and accurate numerical results.[6-11] In higher dimensions numerical[7-11] and functional RG calculations[15,16] show a dependence of the exponents on dimensionality. Accurate determination of their values in simulation studies is often hampered by one or several of the following factors: large intrinsic width of the surface,[7,21] crossover effects,[13,22] and growth oscillations.[23] A crucial step in overcoming these difficulties is to extend the simulation to very large systems.

In this Letter we report a numerical study of a deposition and evaporation model, in an attempt to provide better estimates for the roughness exponents, and to probe the nonequilibrium roughening transition. Using a Potts-spin representation and a multisite-coding, parallel processing algorithm for surface growth, we were able to simulate systems of significantly larger size ($N=L^2=11\,520^2$ sites for $d=2$ and $N=2L^3=2\times192^3$ sites for $d=3$) than most previously reported studies. We give accurate estimates for the roughness exponents which are in conflict with existing conjectures in the literature.[7,11,13,14]

Consider the surface of a stack of hypercubes on a $(11\cdots1)$ substrate plane in $d+1$ dimensions. Such a surface is described by an integral height function $h(\mathbf{x}) \equiv \sum_{\alpha=1}^{d+1} n_\alpha$, where n_α are coordinates of surface site $\mathbf{R}=\sum n_\alpha \hat{\mathbf{e}}_\alpha$ whose projection onto the substrate is given by $\mathbf{x}=\sum n_\alpha \hat{\mathbf{e}}_\alpha^{\parallel}$. A solid-on-solid (SOS) condition on the height $h(\mathbf{x})$ will be assumed at all stages. The model is defined as a sequence of stacking events, each time a hypercube is added to the surface at a deposition rate p^+, or taken away from it at an evaporation rate p^-. It is a generalization of the single-step model considered previously by Plischke, Rácz, and Liu.[9] Using a tiling interpretation, the model describes kinetics of a driven domain-wall system.[24] It can also be viewed as a lattice-gas diffusion model in a *closed* system, with a local updating rule similar to the sand-pile model studied

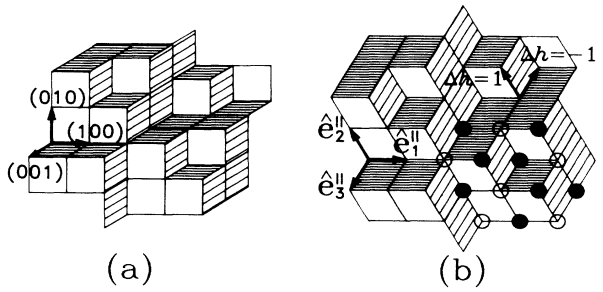

FIG. 1. (a) The surface of a cube stack with only (100), (010), and (001) faces exposed. (b) A rhombus tiling obtained by projection onto a (111) substrate plane. Open ($s=\frac{1}{2}$) and solid ($s=-\frac{1}{2}$) circles indicate Ising spins on vertices (of part) of the tiling. A rhombus edge corresponds to a satisfied antiferromagnetic bond.

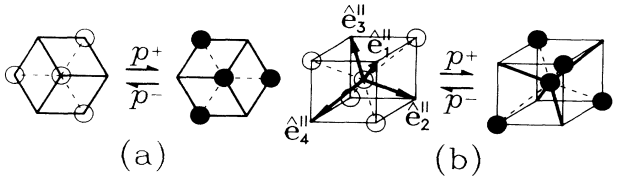

FIG. 2. Local updating rule for the center vertex in (a) $d=2$ and (b) $d=3$ dimensions. Open circles denote Potts spins in state σ, and solid circles, $\sigma+1$ (mod d). Heavy lines indicate satisfied bonds, and dashed lines, unsatisfied bonds. The cubes shown in (b) are a guide to the eye.

by Bak, Tang, and Wiesenfeld.[25]

In addition to the pure deposition case at $p^+=\frac{1}{2}$ and $p^-=0$, which yielded the accurate estimates for the exponents characterizing the rough phase, we studied the model at other values of p^-. Our kinetic model at $p^+=p^-$ generates the distribution for a stationary surface at thermal equilibrium. Indeed, the surface in this case was found to be smooth for $d=3$ and logarithmically rough for $d=2$. For $0<p^-<p^+=\frac{1}{2}$ the situation seems to be different in two and three dimensions. In $d=2$ our results are consistent with the prediction of a transient temporal regime[13] whose size increases rapidly with decreasing p^+-p^-, thus hindering observation of true asymptotic behavior at even a moderate $p^-=p^+/2$. However, our systematic study points to a smooth crossover rather than a sharp nonequilibrium morphological transition in the system. In contrast, the surface-width data in $d=3$ strongly suggests a nonequilibrium roughening transition.[26] Our numerical investigation combined with a known exact result[3] in $d=2$ leads us to conjecture an anomalous scaling form

$$w^2(t)=(\pi K)^{-1}\ln[Lg(t/L^2)]\,, \tag{3}$$

at the roughening transition in our model for $d\geq 2$. Here $g(x)\sim x^{1/2}$ for $x\ll 1$ and becomes a constant for $x\gg 1$, and K is the stiffness constant of the surface when $d=2$.

The mapping from $h(\mathbf{x})$ to the Potts-spin configuration is given explicitly by

$$\sigma(\mathbf{x})\equiv h(\mathbf{x}) \pmod d\,. \tag{4}$$

It can be shown that $\{\sigma(\mathbf{x})\}$ thus obtained is in the ground state of a chiral Potts model with a Hamiltonian $H=-\sum_{\mathbf{x},\alpha}\delta\{\sigma(\mathbf{x})+1,\sigma(\mathbf{x}+\hat{\mathbf{e}}_\alpha^{\parallel})\}$, where $\delta\{i,j\}=1$ if $i=j$ (mod d), and 0 otherwise. Restricting a Potts-spin configuration to be in this class, the SOS condition ensures a unique inverse mapping apart from an overall height shift. Figure 1 shows an example in $d=2$. The rhombus tiling in Fig. 1(b) is the projection of the surface in Fig. 1(a) onto the (111) plane. It is obtained from an Ising-spin configuration $\{s(\mathbf{x})\equiv\sigma(\mathbf{x})-\frac{1}{2}\}$ on the two-dimensional (2D) triangular lattice by simply connecting neighboring sites occupied by opposing spins [see Fig. 1(b)], provided $\{s(\mathbf{x})\}$ is in the antiferromagnetic ground state.[3] The surface height $h(\mathbf{x})$ can be obtained by adding up height differences Δh along rhombus edges or satisfied bonds: $\Delta h=1$ if the edge is oriented along $\hat{\mathbf{e}}_\alpha^{\parallel}$, and $\Delta h=-1$ if it is oriented along $-\hat{\mathbf{e}}_\alpha^{\parallel}$ [see Fig. 1(b)]. For $d=3$ the substrate lattice assumes a body-centered-cubic (bcc) structure.

Our local rule for surface evolution under the SOS condition is illustrated in Fig. 2 for $d=2$ and 3. Deposition $\sigma(\mathbf{x})\rightarrow\sigma(\mathbf{x})+1$ (mod d) at the center vertex is performed, with a probability p^+, if $\sigma(\mathbf{x})=\sigma(\mathbf{x}')$ for all $\mathbf{x}'=\mathbf{x}-\hat{\mathbf{e}}_\alpha^{\parallel}$, $\alpha=1,\ldots,d+1$ (corner sites shown by open circles). Evaporation $\sigma(\mathbf{x})\rightarrow\sigma(\mathbf{x})-1$ (mod d) is performed with a probability p^- under the condition $\sigma(\mathbf{x})=\sigma(\mathbf{x}'')$ for all $\mathbf{x}''=\mathbf{x}+\hat{\mathbf{e}}_\alpha^{\parallel}$, $\alpha=1,\ldots,d+1$ (corner sites shown by solid circles). This local updating rule preserves the ground-state condition on the Potts configuration.

We start from a flat surface at $t=0$, which has an average orientation along the body diagonal $(11\cdots1)$ and a width satisfying $w^2(0)=d(d+2)/12$. Periodic boundary conditions are used in the simulation. A sublattice structure is chosen so that sites on the same sublattice can be updated simultaneously at a given time step. A detailed discussion of the mapping and the growth algorithm will be presented elsewhere.[24]

Our result for the largest systems is summarized in Fig. 3, which shows $w^2(2t)-w^2(t)$ at $p^+=\frac{1}{2}$ and a number of values $p^-=m/64$, plotted against t on a log-log scale. Error bars indicate statistical fluctuations among different realizations. Let us first consider the pure deposition at $m=0$. For both $d=2$ and 3, data approach a straight line at very early times, as in the case of a restricted SOS deposition model studied in Ref. 11. Relative statistical errors on $w^2(t)$, though increasing rapidly during growth, reach only about 0.5% for $d=2$ and about 3% for $d=3$ at the longest time shown. To determine $\beta(d)$, we invoke a convolution *Ansatz*[21] which assumes that the leading correction to Eq. (2) is a size- and time-independent constant. Based on this assump-

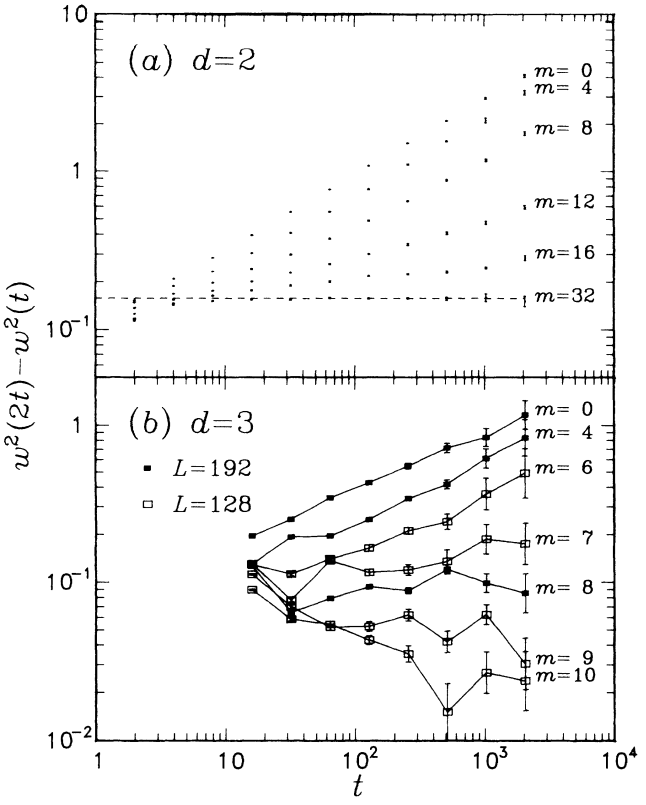

FIG. 3. Surface-width data in (a) $d=2$ and (b) $d=3$ dimensions at $p^+=\frac{1}{2}$ and $p^-=m/64$. Data shown in (a) are for systems of linear size $L=11\,520$ ($m=0$) and $L=5760$ ($m>0$). The dashed line in (a) is at a constant value $9\ln 2/4\pi^2$.

tion, we performed a linear least-squares analysis to (i) $\ln[w^2(t)-w_0^2]=2\beta\ln t+\text{const}$, and (ii) $\ln[w^2(2t)-w^2(t)]=2\beta\ln t+\text{const}$. The constant $w_0\simeq w(0)$ is chosen to extend the plateau of the fitted slope to shorter times. The exponent $\beta(2)$ thus obtained is listed in Table I. Numbers in parentheses give the uncertainty in the last digit from a standard regression analysis. The fitted slopes at large t show an excellent agreement with

TABLE I. Successive estimates of the dynamical exponent β.

	$\beta(2)$ [a]		$\beta(2)$ [b]	
t	$M=3$	$M=4$	$M=3$	$M=4$
4	0.245(3)	0.243(2)	0.230(6)	0.233(3)
16	0.2402(2)	0.2399(2)	0.241(2)	0.2406(8)
64	0.2403(6)	0.2405(3)	0.242(2)	0.240(2)
256	0.2400(3)	0.2401(2)	0.240(2)	0.2400(8)
1024	0.2403(2)			

[a]From $\ln[w^2(t)-w_0^2]$ vs $\ln t$ at M consecutive times $t, 2t, \ldots, 2^{M-1}t$.

[b]From $\ln[w^2(2t)-w^2(t)]$ vs $\ln t$ at M consecutive times $t, 2t, \ldots, 2^{M-1}t$.

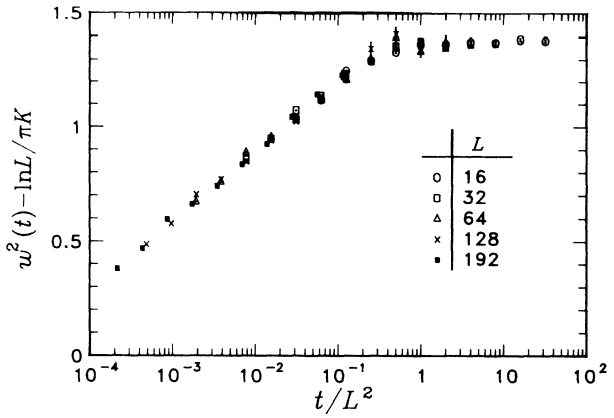

FIG. 4. A scaling plot of surface-width data in three dimensions at $p^+=\frac{1}{2}$ and $p^-=\frac{1}{8}$ using $K=1.2$.

each other, and yield $\beta(2)=0.240\pm0.001$. Because of a smaller linear system size and growth oscillation at short times, our estimate for $\beta(3)=0.180\pm0.005$ is less accurate. We also determined the exponent $\zeta(2)=0.385\pm0.005$ and $\zeta(3)=0.30\pm0.01$ using a steady-state surface width in systems up to $L=480$ in $d=2$ and $L=128$ in $d=3$, respectively. The relation $\zeta+z=2$ is satisfied in both cases within our numerical accuracy.

Focusing on Fig. 3(a) for $d=2$, the equilibrium case ($m=32$) reaches a plateau around $\ln 2/2\pi K$ (shown by the dashed line), thus confirming (3). Here $K=2\pi/9$ is the exact value determined in Ref. 3. Data in between the equilibrium and pure deposition ($m=0$) case show a crossover behavior. The time which it takes to reach the asymptotic regime grows rapidly with increasing m, and goes beyond our longest simulation time at $m=16$ or $p^-=p^+/2$. Simulations at p^- closer to p^+ in systems even as large as ours and over a broad time range may very well yield an effective exponent β_{eff} lower than the asymptotic value. Our result at different values of m show that it might be misleading to interpret a change in β_{eff} as an indication of a kinetic morphological transition.

A different situation is encountered in Fig. 3(b) for $d=3$. Data at large t increase with t for $m\leq 7$ and decrease for $m\geq 9$, while remaining approximately constant at $m=8$. This suggests a nonequilibrium roughening transition at $p^-=p_c^-=\frac{1}{8}\pm\frac{1}{64}$. We also studied the behavior of $\omega^2(t)$ below the transition at $m=12$ and 16 (not shown). Both cases exhibit the same behavior as a smooth surface at equilibrium. The width of the surface saturates to a constant with a $1/L$ correction.[24]

Figure 4 shows scaled $w^2(t)$ data at $m=8$ and a number of system sizes from $L=16$ to 192 on a semilog plot, using $K=1.2$. There appears to be a good agreement between the data and the conjectured anomalous scaling form (3) over the time range and system sizes studied. This in addition gives a confirmation of the transition point $p_c^-\simeq\frac{1}{8}$ determined above.

In conclusion, we have presented a detailed numerical

study of a hypercube-stacking model which includes both deposition and evaporation processes. Accurate estimates for the exponents characterizing the rough phase of the model were given. We studied the nonequilibrium roughening transition in three dimensions, and proposed an anomalous scaling form for the surface width at the transition.

The height-height correlation function of our model can be directly related to a four-spin-correlation function in the Potts-spin representation.[3] Thus it should be possible to study the behavior of the rough phase and the nonequilibrium roughening transition by looking at appropriate order parameters of the Potts-spin system. Another feature of our model is an intrinsic sublattice structure associated with the layering of $(11\cdots1)$ lattice planes of the $(d+1)$-dimensional hypercubic lattice. Our preliminary studies[24] in $d=3$ indicate that the average height of different sublattices is different in the smooth phase, but becomes the same in the rough phase (apart from a finite-size correction). The vanishing of the difference in the average heights appears to take place right at the roughening transition. It would be interesting to further explore this apparent coincidence.

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