Reconstructed rough growing interfaces: Ridge-line trapping of domain walls

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We investigate whether surface reconstruction order exists in stationary growing states at all length scales or only below a crossover length $l_{\rm rec}$. The latter behavior would be similar to surface roughness in growing crystal surfaces; below the equilibrium roughening temperature they evolve in a layer-by-layer mode within a crossover length scale $l_{\rm R}$, but are always rough at large length scales. We investigate this issue in the context of Kardar-Parisi-Zhang (KPZ) type dynamics and a checkerboard type reconstruction, using the restricted solid-on-solid model with negative monatomic step energies. This is a topology where surface reconstruction order is compatible with surface roughness and where a so-called reconstructed rough phase exists in equilibrium. We find that during growth reconstruction order is absent in the thermodynamic limit, but exists below a crossover length $l_{\rm rec}>l_{\rm R}$, and that this local order fluctuates critically. Domain walls become trapped at the ridge lines of the rough surface, and thus the reconstruction order fluctuations are slaved to the KPZ dynamics.

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I. INTRODUCTION

Equilibrium surface phase transitions have been a topic of research for several decades. Various types of critical behavior are well established in both theoretical models and actual experiments. This topic includes surface roughening [1,2], surface melting [3,4], and surface reconstruction [5–7]. Moreover, the competition between these phenomena leads to additional phases and phase transitions, like disordered flat phases, preroughening transitions, and reconstructed rough phases [8–10]. Roughening induced deconstruction in Pt(110) [7,11] and preroughening induced deconstruction in Si(110) type geometries are other examples of this competition [12].

The theory of dynamic nonequilibrium processes like surface growth has flourished during the last decade as well. Several additional types of dynamic universality class have been identified. Kardar-Parisi-Zhang (KPZ) type growth is one example [13–20]. Unfortunately, in this area the gap seems wider between theoretical and experimental interests. Theoretically oriented research tends to focus on universal aspects of these processes, such as the large scale properties of growing surfaces in the stationary growing state and how this state is approached in the asymptotic large time limit. Experimentally oriented research tends to focus on more microscopic short distance aspects of growing surfaces, e.g., as encountered in actual epitaxial growth.

One of the fundamental issues relevant to both perspectives is whether any of the above equilibrium surface phase transitions persist in the stationary state of growing interfaces. In this paper we address whether surface reconstruction order can exist during growth.

This issue is related to the absence of surface roughening transitions in growing surfaces. Below the equilibrium roughening transition temperature $T_{\rm R}$ the growing surface is rough at large length scales, but remains flat and grows layer by layer at distances shorter than a crossover length scale $l_{\rm R}$, which varies with temperature and oversaturation. We review this briefly in Sec. II in the context of elementary nucleation theory.

Consider a surface that is flat and reconstructed in equilibrium at low temperatures. Below $T_{\rm R}$ it appears to grow within $l_{\rm R}$ as flat in a layer-by-layer mode. Moreover, below $T_{\rm rec}$ (if $T_{\rm rec}<T_{\rm R}$) it appears as reconstructed if the new particles can find their proper reconstruction positions at time scales that are short compared to the rate at which a new layer is completed. Presume that this is indeed the case. The next, more intriguing, question is whether $l_{\rm rec}$ can be larger than $l_{\rm R}$; i.e., whether rough growing surfaces can be reconstructed? The compatibility of surface roughness with surface reconstruction was addressed in the context of equilibrium phase transitions several years ago. The answer depends on intricate details of the surface topology. For example, in missing row reconstructed (MRR) (110) facets in fcc crystals, like Au and Pt, roughness is incompatible with reconstruction order, and the surface roughening transition must simultaneously destroy the reconstruction [7]. In such geometries, reconstruction order cannot exist in growing surfaces beyond the roughness length scale either, and $l_{\rm rec}\leqslant l_{\rm R}$.

Surface roughness and reconstruction are compatible with each other in other crystal structures. Simple cubic (sc) MR reconstructed (110) facets are an example. In equilibrium, they can roughen before the reconstruction order deconstructs, $T_{\rm R}<T_{\rm rec}$. The intermediate phase is known as a reconstructed rough phase [7,10]. For those surfaces it might be possible to observe genuine deconstruction type phase transitions in growing surfaces. Or, if not, the surface reconstruction can at least persist well beyond the roughness crossover length scale, $l_{\rm rec}>l_{\rm R}$, and will be limited by an independent mechanism. These issues are the topic of our research reported here.

In Sec. II we review rough versus layer-by-layer growth in surfaces, and in Sec. III the basic properties of equilibrium reconstructed rough phases. Next, in Sec. IV, we start to focus on the reconstruction versus dynamic roughness issue, and then, in section V, we choose a specific type of reconstruction and a specific type of surface growth dynamics to study it quantitatively by means of Monte Carlo (MC) simulations. The model must be as simple as possible, avoiding

secondary effects that might obscure the central issue. Our choice is the so-called restricted solid-on-solid (RSOS) model with negative step energies, which describes a simple cubic checkerboard type reconstruction, and KPZ type growth. The MC simulation results are presented in Sec. VI, and analyzed in Sec. VII. Finally, in Sec. VIII we summarize our results.

II. ROUGHNESS IN GROWING SURFACES

The topic of this paper is whether surface reconstruction order can exist during growth, but as a start it is useful to review briefly the related issue of dynamic surface roughness from long and short length scale perspectives. Elementary nucleation theory suffices for this purpose. Equilibrium crystal surfaces undergo well defined roughening transitions from macroscopic flat to macroscopic rough. On the other hand, growing surfaces are theoretically ''always rough'' [21,22]. This seems at odds with practical reality, where surfaces appear to grow quite differently below and above the equilibrium roughening temperature T_R. Above T_R they are rough (dynamic roughness) while below T_R they seem flat (layer-by-layer growth on flat surfaces as well as step-flow growth on sloped ones [23,24]). Above T_R the growth velocity v_g is proportional to the oversaturation $v_g \sim \Delta\mu$, while below T_R it is inversely proportional to a nucleation time scale $v_g \sim \tau^{-1}$ with $\tau^{-1} \sim \exp[-a\eta^2/(\Delta\mu k_B T)]$ [21]. η is the equilibrium step free energy. As a result, crystal growth shapes have sharp angles, in which many facets, including all that are above their T_R, are missing. This apparent difference in growth mechanism is one of the most useful experimental tools to locate equilibrium roughening transitions in crystal facets.

The origin of the exponential factor in τ is the existence of a nucleation barrier for creating a terrace of height $h \rightarrow h+1$ below T_R. The edge (step) free energy loss term (proportional to η times the circumference) competes with the surface energy gain term (proportional to $\Delta\mu$ times the terrace area). The nucleation barrier vanishes when the step free energy η vanishes, i.e., at T_R. After a new terrace larger than the nucleation threshold is nucleated with an exponentially small probability, it spreads out fast by particle adhesion at its edge into a macroscopic domain, until it merges with other spreading terraces that have nucleated in the mean time, and thus completes the new surface layer. However, new terraces are nucleated on top of spreading terraces as well. This nesting effect, together with the spatial fluctuations of nucleation events, leads to the loss of a well defined (length scale free) global reference surface level. This means that, although at small enough length scales the surface looks flat and seems to grow layer by layer, at large length scales it is rough.

There is no phase transition between the layer-by-layer and rough growth regimes, only a characteristic crossover length scale. The latter is of order $l_R = v_s \tau$, with v_s the step velocity (determined by the particle deposition rate at the step edge) and τ the above time scale at which terrace nuclei are being created. Surface flatness cannot be maintained during growth over large length scales, but at small oversaturations ($\Delta\mu$) and sufficiently below T_R (large step free energies η) the growing surface can appear to be flat for all practical purposes, over any typical experimental length scale.

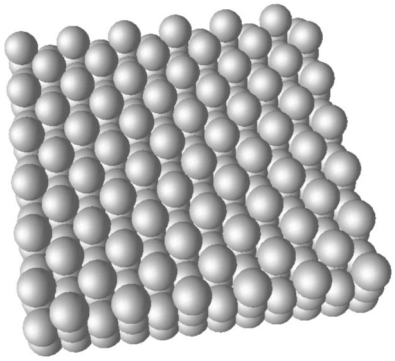

FIG. 1. checkerboard type misplacement surface reconstruction.

The same types of issue arise in our study concerning the compatibility of surface reconstruction order with growth dynamics. First we address whether surface reconstruction order can persist during growth at macroscopic length scales (the thermodynamic limit); and, if not, whether it might still exist in a practical sense within a characteristic length scale l_{rec} below the equilibrium reconstruction temperature T_{rec}.

III. RECONSTRUCTED ROUGH EQUILIBRIUM PHASES

Surface reconstruction is conventionally associated with flat interfaces. However, surface roughness does not necessarily destroy the reconstruction order. A rough but still reconstructed surface is in a so-called reconstructed rough (RR) phase. The equilibrium versions of RR phases were studied theoretically some years ago in the context of the competition between surface roughening and reconstruction in MR reconstructed fcc (110) facets [6,7]. The topological details of those fcc surface prevent the existence of RR phases, implying that in Pt(110) the surface roughens and deconstructs simultaneously [7] as observed experimentally in Pt(110) [11]. This implies immediately that during growth reconstruction order is limited to the roughness crossover length scale, $l_{rec} \leqslant l_R$. The same theoretical studies also identified other surface geometries where RR phases do exist. For those l_{rec} is not limited by l_R. In this section we review the basic properties of RR phases, using as examples checkerboard and MR type reconstructed simple cubic stackings.

To avoid confusion, it is useful to distinguish between misplacement and displacement type reconstruction [10]. In misplacement reconstructions, particles have moved to different solid-on-solid type stacking positions, or are removed altogether, compared to the unreconstructed flat surface structure. The checkerboard reconstruction in Fig. 1 and also the more realistic MR type reconstructions are examples of this. The average surface height has changed by half a unit, $h \rightarrow h - \frac{1}{2}$. In displacement reconstructions the atomic stacking does not change. Instead, the atoms are merely elastically distorted at the surface with a commensurate or incommensurate period compared to the bulk. Misplacement type re-

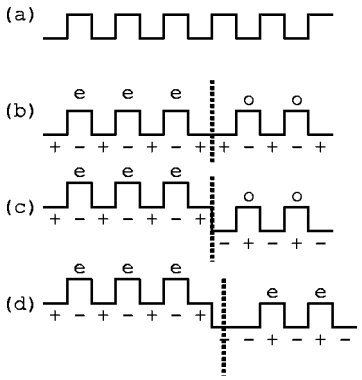

FIG. 2. (a) A perfect reconstructed surface. (b) A domain wall; both order parameters change sign. (c) A step where only the even-odd row order changes sign. (d) A step where only the parity order changes sign.

constructions are more likely to disorder at temperatures near T_R than displacement type reconstructions. For clarity we focus here on misplacement reconstructions.

The definition of the reconstruction order parameter is at the core of RR phases [7,10]. In checkerboard and MR reconstructed sc (110) facets, the reconstruction order can be formulated in two distinct ways. One formulation keeps track of whether the black or white field (even or odd row) is on top. The other measures it in terms of antiferromagnetic order in the parity type Ising variables $S_r = \exp(i\pi h_r)$, with $h_r = 0, \pm 1, \pm 2, \ldots$ the surface height at site r (see Fig. 2). These two formulations might seem equivalent in flat surfaces, but they are not in the presence of roughness.

The compatibility of surface reconstruction with surface roughness depends on topological properties of step and domain wall excitations; on how they affect the two versions of the order parameter. Figure 2 shows in cartoon style a cross section of the reconstructed surface, and also domain wall and step excitations. The domain wall in (b) does not change the surface height. Notice that both order parameters change sign. Across the step in (c), from left to right, the even-odd order parameter changes sign, but the parity order is unaffected. At the step in (d) the opposite happens. These two types of step are the only topologically distinct ones that are possible; (c) couples only to the even-odd row type order parameter and (d) only to to the parity version.

It is possible to construct many more step and domain wall structures that look locally different from the ones in the figure, but those induce the same change in height and/or reconstruction order(s) and therefore are from a topological point of view identical to the ones in the figure. Notice also that the excitations in (b)–(d) are related to each other in the sense that any of the three can be interpreted as a bound state of the two others. Elastic surface deformations in the actual atomic positions near the surface and additional ones near the steps and domain walls influence the local internal structure of steps and domain walls, but do not affect these topological features, and therefore need not be explicitly represented in the following discussion. (They certainly renormalize the step and domain wall energies and the interactions between such surface excitations.)

The fate of reconstruction versus roughness depends on the energies of these steps and domain walls, including the kink energies. They set the scale of the meander type entropy and therefore the temperature dependence of the step free energies. If the domain wall free energy vanishes first, the surface remains flat but the reconstruction vanishes, $T_{rec} < T_R$. In case the free energy of one of the two types of step vanishes first, the surface enters a reconstructed rough phase, $T_R < T_{rec}$. At the roughening transition one of the two reconstruction order parameters vanishes, but the other type of order remains. So there exist two topologically distinct types of RR phase. (Notice that only the one with the parity type order is readily observable by, e.g., conventional x-ray diffraction.)

In the RSOS model below, the RR phase has parity order, i.e., the step free energy of the (c) type steps is zero, but walls and (d) type steps still have nonzero free energy. We will refer to those excitations as ''loops of zeros,'' because in the rough surface they show up as contours across which the height change is zero, $dh = 0$. The deconstruction transition (inside the rough phase) takes place at the temperature where the surface tension of the loops vanishes. In equilibrium that turns out to be an ordinary Ising transition. This concludes our brief review. For more details we refer to Refs. [7] and [10].

IV. RECONSTRUCTED ROUGH GROWTH

Let us focus now on surface growth. Only in surfaces where equilibrium RR phases are topologically possible can the surface reconstruction length scale l_{rec} exceed the onset of dynamic roughness of length scale l_R. Moreover, it is quite possible that the reconstruction order persists over all length scales ($l_{rec} \to \infty$), such that a genuine dynamic deconstruction phase transition takes place in the stationary state of the growing surface, just as in equilibrium.

For comparison, imagine a two-dimensional (2D) lattice with a height variable and an Ising spin degree of freedom (representing the reconstruction order) on each site. This leads to two coupled master equations, one for surface growth, e.g., KPZ type dynamics, and the other for the reconstruction order, e.g., Glauber type Ising dynamics. In equilibrium surfaces, the coupling between the two sectors is weak, to the extent that the reconstruction transition in the Ising sector and the roughening transition in the height variable sector do not interfere with each other [7,25]. The central issue is whether and how this coupling changes during growth. The Ising dynamics itself is blind to the growth bias. If the coupling between the two sectors remains weak, the Ising spins can still reach the Gibbs equilibrium state and undergo a conventional equilibrium reconstruction transition.

Coupled master equations of this type have been studied recently in the context of specific 1D growth models. Those display strong coupling between the Ising and roughness degrees of freedom, such as growth being pinned down by Ising domain walls [26–28]. Pinning favors spontaneous faceting. In our 2D model, we observe different effects, in addition to the obvious fact that in 1D equilibrium reconstruction order cannot exist.

V. RESTRICTED SOLID-ON-SOLID MODEL

The 2D restricted solid-on-solid model is one of the work horses of surface physics research. Integer valued height variables $h_r = 0, \pm 1, \pm 2, \ldots$ are assigned to a square lattice and nearest neighbor heights are restricted to differ by at most one unit, $dh = 0, \pm 1$. The energy

$$E = \frac{1}{2} K \sum_{\langle r,r' \rangle} (h_r - h_{r'})^2 \tag{1}$$

depends only on nearest neighbor interactions. We use dimensionless units, $K = J/k_B T$. The $K > 0$ side of the phase diagram contains a conventional equilibrium surface roughening transition [25]. Moreover, the nonequilibrium version has been studied extensively for $K > 0$ as well, because it is a natural lattice realization of KPZ growth [13–19].

For $K < 0$, the model contains one of the simplest examples of an equilibrium RR phase [25], and is probably the most compact formulation of the coupling between Ising and surface degrees of freedom. The $dh = \pm 1$ steps are more favorable than flat $dh = 0$ segments. At zero temperature, $K \to -\infty$, the $dh = 0$ states are frozen out, and the model reduces to the so-called body centered solid-on-solid (BCSOS) model, but in this version it lacks step energies, which means that the surface is rough even at zero temperature. The surface is rough, but since nearest neighbor heights must differ by 1, all heights on one sublattice are even, and odd on the other, or the other way around. This two-fold degeneracy represents the checkerboard type RR order. The staggered magnetization, defined in terms of the parity spin type variables $S_i = \exp(i\pi h_r)$, is nonzero.

The $dh = 0$ excitations that appear at $T > 0$ form closed loops and behave like Ising type domain walls. The reconstruction order changes sign across such loops. Their sizes diverge at the equilibrium deconstruction transition $K_c = -0.9630$ [25] (determined by transfer matrix finite size scaling techniques). The Ising and roughness variables couple only weakly. Numerically, all reconstruction aspects of the transition follow conventional Ising critical exponents. Moreover, the thermodynamic singularities in the Ising sector affect only the temperature dependence of the surface roughness parameter K_G, defined in terms of the height-height correlator,

$$\langle (h_{r+r_0} - h_{r_0})^2 \rangle \simeq (\pi K_G)^{-1} \ln(r). \tag{2}$$

The continuum limit analysis confirms these numerical results. The point in the generalized phase diagram where the Gaussian (height) and Ising degrees of freedom decouple is a stable renormalization type fixed point [10].

We study this same RSOS model in the presence of a KPZ type growth bias. In the MC simulation, we first select an update column and next whether a particle deposition or evaporation event will be attempted. The move is rejected if it would result in a violation of the RSOS condition $dh = 0, \pm 1$. If allowed, it will take place with probability $P = \min(p, pe^{-\Delta E_j})$ in case of deposition, and with probability $P = \min(q, qe^{-\Delta E_j})$ for evaporation. Without loss of generality we can choose $p + q = 1$. At infinite temperature ($K = 0$) and deposition only ($q = 0$) the model reduces to the well known Kim-Kosterlitz [18] model for KPZ type growth.

We will present only our MC results far from equilibrium, i.e., at $q = 0$ with deposition only. We observe no qualitative differences closer to equilibrium, $0 < p < 1$, but the interpretation of the data becomes increasingly obscured (as expected) by (conventional) crossover scaling from the equilibrium deconstruction phase transition.

At low temperatures, $K \to -\infty$, the Metropolis dynamics slows down considerably. The rejection rate becomes high and the density of active sites becomes low. Therefore we employ the following rejection free algorithm. During the MC simulation we keep a list of active sites, i.e., sites where particles can deposit without violating the RSOS condition. They are grouped in $j = 1, \ldots, 5$ sets, according to the five distinct energy changes ΔE_j that can occur during deposition. First we preselect one of those five sets, with probability $(p_j N_j)/(\Sigma_j p_j N_j)$, where $p_j = \min(1, e^{-\Delta E_j})$ and N_j is the number of sites of type j. Next, a particle is randomly deposited at one of the sites in that specific set j. Rejection free procedures like this upset the flow of time. To restore proper time, we increase the MC time during each update step by $1/p \times 1/N_j$. We checked explicitly that this reproduces the correct value for the KPZ dynamic exponent $z = 8/5$ [18–20] at $K \simeq 0$; we find $z \simeq 1.6 \pm 0.1$.

The above algorithm resolves the slowing down problem in the actual MC simulation, but does not address its origin. In the limit $K \to -\infty$ the RSOS model reduces to the BCSOS model, with $dh = \pm 1$ at all bonds. The $dh = 0$ loops are frozen out completely. In BCSOS type KPZ growth dynamics, two particles are deposited at once in the form of vertically oriented bricks, otherwise a ''forbidden'' configuration with $dh = 0$ would arise. In the $K < 0$ RSOS model at very low temperatures the same event is achieved as a two-step two-particle process, by the deposition of a second particle at the same site soon after the first one. The probability for deposition of the first particle is equal to $p = L^{-2} \exp(2K)$. The second particle deposition on top of it happens with probability $p = L^{-2}$. This implies that the time clock in the RSOS model runs more slowly by a factor $r = \exp(2K)[1 + 4\exp(K) + \cdots]$.

A final remark about surface roughness. In normal surfaces, the equilibrium roughness increases with temperature, due to the fact that meander type entropy renormalizes the step energy into a reduced step free energy [10]. In our model, surface roughness evolves in the opposite way; it decreases with increasing temperature. The surface is less rough at infinite temperature $K = 0$ than in the zero temperature limit $K \to -\infty$. A high temperature RSOS surface, with $dh = 0, \pm 1$ is obviously less rough than a BCSOS surface, with only $dh = \pm 1$. Recall that this BCSOS model lacks step energies, such that it is just as rough at $T = 0$ as at $T \to \infty$. From the BCSOS perspective the thermally excited $dh = 0$ loops stiffen the surface, and give rise to an inverted roughness versus temperature profile. On the one hand, this is an interesting phenomenon in its own right. Moreover, we could fine tune it by introducing next-nearest neighbor interactions, since they represent BCSOS type step energies. On the other

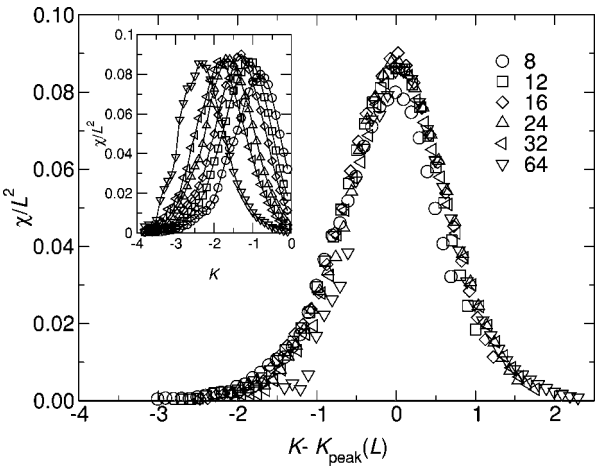

FIG. 3. Reconstruction order susceptibility χ as function of temperature at system sizes $L=8-64$. The data collapse onto a single curve by the shift $K'=K-K_{\mathrm{peak}}(L)$, with $K_{\mathrm{peak}}(L)=-0.77\ln(L/2.2)$.

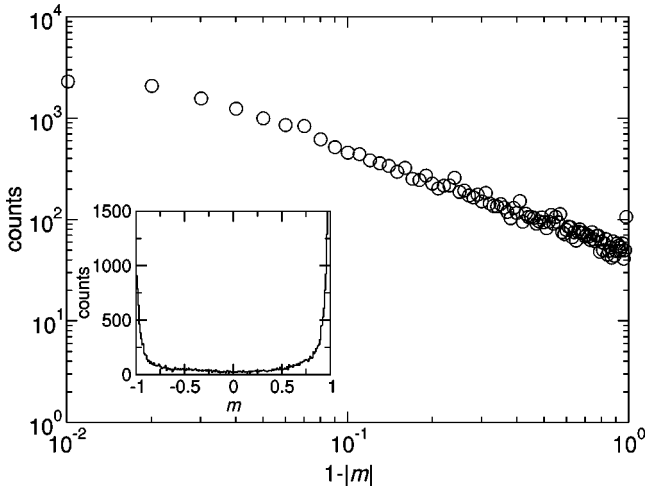

FIG. 4. Histogram (inset) of the reconstruction order parameter m at $L=32$ and $K=-3.2$ from 2^{18} data points using $\Delta M=0.01$ as bin width. The tails about the peaks at $m=\pm 1$ scale as power laws (main frame) with exponent -0.9 ± 0.1.

hand, this effect is unlikely to affect the central question we want to address (how do roughness and reconstruction degrees couple during growth) and therefore we choose not to do so in this study.

VI. RECONSTRUCTION DURING GROWTH

We search for reconstruction order as a function of temperature, for $-\infty<K<0$. The susceptibility type parameter [29]

$$\chi=L^2(\langle m^2\rangle-\langle|m|\rangle^2) \tag{3}$$

of the reconstruction order parameter

$$m=\langle(-1)^{x+y}e^{i\pi h(x,y)}\rangle \tag{4}$$

is shown in Fig. 3 for the stationary state of the growing surface, as a function of K for different system sizes L^2. The sharp maxima seem to confirm the existence of a dynamic surface reconstruction transition into a RR phase. However, several features are very different from equilibrium. The peak height diverges as $\chi\sim L^2$; i.e., more strongly than at the equilibrium transition point where it scales as $\chi\sim L^{\gamma/\nu}$. This could be a signal of a first order phase transition. However, the peak position does not converge to a specific critical point K_c. Instead it keeps shifting with lattice size. It scales logarithmically, as $K_{\mathrm{peak}}(L)\simeq -A\ln(L/L_0)$ with $A=0.77\pm 0.05$ and $L_0=2.2\pm 0.2$.

Next, we monitor in detail the reconstruction order parameter m near and below the equilibrium K_c as a function of time. It behaves similarly as in conventional spontaneously ordered phases, but flipflops more frequently than is justifiable from finite size effects alone. Moreover, the fluctuations in m within each phase are too strong. Figure 4 quantifies this in terms of a histogram of the number of times a specific value of m appears in a typical time series. The distribution has two distinct peaks, suggesting the presence of spontaneously broken reconstruction order, but the tails have a power law shape instead of the exponential form mandatory for a spontaneously broken symmetry.

Power laws are the hallmark of critical fluctuations. So, quite surprisingly, it appears as if the RR order is critical at low temperatures for all $K<K_{\mathrm{peak}}$. Instead of an isolated critical point, we seem to be dealing with a critical phase.

VII. LOOPS TRAPPED ON RIDGE LINES

The surprising critical fluctuations in the reconstruction order parameter can be traced to the following loop dynamics. Consider a typical configuration at very low temperatures. Figure 5 shows an example [30]. The surface is in an almost pure BCSOS type dynamic rough stationary state (with $dh=1$), and contains only a few $dh=0$ loops separating surface areas of opposite checkerboard type RR order.

The typical life cycle of such a loop runs as follows. It is nucleated in a valley bottom. Next it runs up hill, growing in diameter and encompassing the entire valley, until it becomes trapped on a ridge line. There it lingers until another

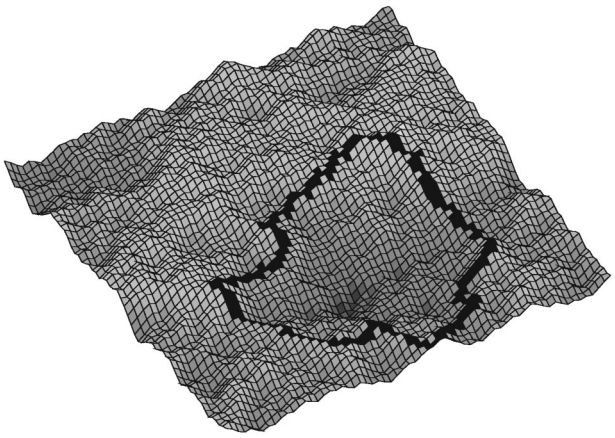

FIG. 5. A typical low temperature configuration of the growing surface with one large loop trapped at a ridge line.

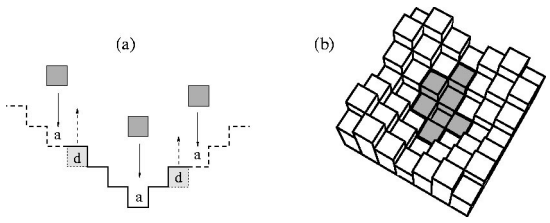

FIG. 6. (a) One-dimensional cross section of the surface near a valley with two loop segments. On the slope, a (d) are the only active adsorption (desorption) sites. The domain walls always move upward during adsorption. (b) A loop of size of l_c nucleated at the bottom of a local valley. Gray and white sites have different surface reconstruction parity order.

loop annihilates it, or until the KPZ surface fluctuations to which it is slaved shrink it back to zero.

Figure 6(a) represents a cross-section of the 2D rough surface near a valley. It shows a domain of opposite reconstruction inside an otherwise perfectly reconstructed rough configuration. The two flat segments are the locations where the domain wall loop intersects the cross section. In equilibrium, the loop fluctuates with equal probability up and down the slope because depositions and evaporations are equally likely. A growth bias breaks this symmetry, the loops more likely move upward than downward, [see Fig. 6(a)]. This upward drift is the driving force responsible for the trapping of loops at ridge lines, and thus creates a strong coupling between the roughness and reconstruction degrees of freedom, unlike equilibrium where they effectively decouple.

A few comments on the topology of ridge lines in rough surfaces might be useful. Imagine a rolling ball in this landscape, as in the well known analogy with renormalization flow in statistical physics. Presume strong friction such that the velocity is proportional to the force, i.e., the gradient of the slope, at all times. The hilltops are the completely unstable ''fixed points.'' The valleys are the attractors. The ridge lines form the watersheds between valleys. Every ridge line runs from a hilltop to a saddle point. From each hilltop an arbitrary number of ridge lines can emerge, but only two ridge lines can end at each saddle point (at opposite sides of the single direction in which the saddle point attracts). So the ridge lines form a network, and since none of them can stop in midair it is a closed network. The KPZ rough surface is scale invariant, which means that this ridge-line network has fractal properties.

Ignore, for the time being, the scale invariant aspects of the network. Imagine a landscape consisting of deep smooth valleys surrounded by ridge lines, unlike the real rough surface where every deep valley consists of collections of subvalleys. The life cycle of a macroscopic loop in this surface starts with the nucleation of a new seedling loop at the floor of the valley and its rise along the slopes, during which it grows into a macroscopic object. The only loops of interest are those nucleated at the valley bottom and then running uphill encompassing the entire valley. Only those loops are topologically trapped and stable. Loops nucleated on the slopes annihilate by stochastic fluctuations before becoming macroscopically large. The same is true for loops nucleated out of the valley bottom but running uphill on one slope segment only.

The rise of a seedling loop out of the valley bottom into a macroscopic object is a very fast process. Almost no MC moves that make the loop grow and rise are rejected; energy barriers are rare, because the length of the loop (its energy) increases uniformly. Compared to this, the nucleation frequency in the valley bottom is very small. This means that the time scale at which a macroscopic loop emerges out of the valley is limited by the nucleation time scale τ_n and independent of the valley size.

To measure τ_n we prepared a surface in the BCSOS KPZ stationary state and measure (at a very low temperature, $K \ll K_c$) the intervals between macroscopic loop events. Numerically we find $\tau_n \sim \exp(-\alpha K)$ (measured in BCSOS time units) with $\alpha = 3.0 \pm 0.1$.

This agrees qualitatively with the following estimate. The deposition of the first particle in the valley bottom occurs with probability $p = L^{-2} e^{2K}$. This creates a fledgling loop, but one that is indistinguishable from the intermediate state in an elementary BCSOS type growth event (where a second particle is dropped on top of it with probability $p = L^{-2}$). The loop grows when the next particle is dropped not on top but next to the previous one. That happens with probability $p = L^{-2} e^{K}$. The nucleation threshold diameter l_c is reached when the loop growth and BCSOS growth become distinguishable, i.e., when the annihilation of a loop requires the creation of a new easily distinguishable loop inside it. That happens at about $l_c^2 \simeq 7$ [see Fig. 6(b)]. The time scale at which that stage is reached is approximately $\tau \simeq L^{-2} e^{-4K}$ (in BCSOS time units), which is of the same order of magnitude as the above numerical nucleation time scale.

The loop rises out of the valley until it becomes trapped on the ridge line that separates this valley from adjacent ones. From there on the loop is slaved to the growth fluctuations of the surface. Valleys grow and shrink (without bias), open up, fill up, and merge. The loop has to follow this dance of the ridge line until a new loop nucleates out of the valley and annihilates it, or until the encircled terrain happens to shrink to zero (fills up) by surface growth fluctuations.

We expect that the lifetime $\tau_z(L)$ of a ridge line of size L in a growing surface scales as a power law $\tau_z \sim L^z$, with z the dynamic exponent of the surface roughness degrees of freedom (KPZ like in our model). To test this, we measure the decay times of large macroscopic defect loops (of about half the lattice size) as a function of L, at low temperatures $K \ll K_c$. The data in Fig. 7 indeed collapse onto one universal curve after a rescaling of time by $\tau_z \approx L^z$. The collapse fits best at $z = 1.7 \pm 0.1$ (in BCSOS time units), which is consistent with the known KPZ dynamical exponent $z = 8/5$ [18–20].

The ridge-line fluctuations are responsible for the power law tails in the time distribution of RR order, Fig. 4. Those critical fluctuations show up only below a characteristic length scale l_{rec}, where the nucleation time scale $\tau_n \sim \exp(-\alpha K)$ is larger than the surface growth time scale $\tau_z \sim L^z$. A simple estimate for l_{rec} follows from equating the two time scales, $l_{\mathrm{rec}} \sim \exp(\alpha K/z)$.

The peaks in the susceptibility in Fig. 3 reflect this cross-

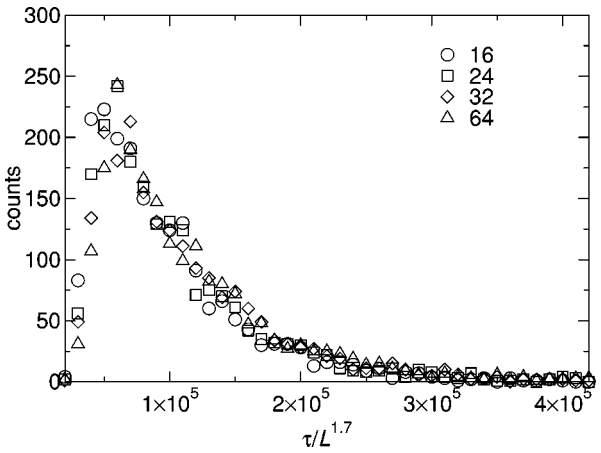

FIG. 7. Histogram of the decay time of a trapped loop at $K=-6.0$. The data collapse by rescaling time by a factor $L^{1.7}$.

over length l_{rec}. Recall that the peak shifts logarithmically. By setting $\tau_n=\tau_z$ we obtain the same logarithmic behavior, $K_{\mathrm{c}}=-(z/\alpha)\ln(L/L_0)$. The prefactor is too small by about 30%, but this is not a surprise because the estimate is rather simple minded. It ignores, for example, the self-similarity of the rough surface. Consider a subvalley adjacent to an already trapped loop. Suppose a new loop nucleates out of this subvalley. The loop segments annihilate each other in pairs. The net effect of this nucleation event is therefore that the trapped loop jumps across the sub valley. It now follows the complementary segment of the ridge line that encircles the subvalley. Such events renormalize τ_z, in particular near K_{c}.

VIII. CONCLUSIONS

In this paper we study the compatibility of surface reconstruction and surface roughness during growth. There are several possibilities.

In surfaces where reconstructed rough phases are topologically forbidden, like missing row reconstructed fcc (110) facets, reconstruction order cannot exist on a global scale in the stationary growing state. It can appear only locally within the crossover roughness length scale l_{R} within which the surface grows in a layer-by-layer fashion, i.e., $l_{\mathrm{rec}}\leqslant l_{\mathrm{R}}$. The reconstruction length scale l_{rec} can exceed l_{R} only in surfaces where equilibrium reconstructed rough phases are topologically possible, and those surfaces could in principle even display genuine deconstruction type phase transitions in the stationary growing state.

We address this issue in the context of KPZ type dynamics, in the RSOS model with negative coupling constant $K<0$, which in equilibrium has a checkerboard type RR phase and a true deconstruction phase transition inside the rough phase. We find that the stationary growing rough state lacks true macroscopic RR order; l_{rec} remains finite. Moreover, we identify the mechanism that sets the temperature dependence of l_{rec}.

The fundamental features are an upward drift of the reconstruction domain wall loops and their trapping at the ridge lines of the surface. There, the loops are slaved to fluctuations of the surface growth dynamics. l_{rec} is set by the competition between two time scales: the nucleation time scale of a new loop out of the valleys (annihilating existing trapped loops) and the time scale $\tau_{KPZ}\sim L^z$ at which a ridge line of radius L vanishes due to surface growth fluctuations.

At length scales smaller than $l_{\mathrm{rec}}\sim\exp(\alpha K/z)$, the surface appears as reconstructed rough, and the lifetime of the loops is determined by the KPZ growth dynamical fluctuations. The latter follow power laws. This manifests itself in critical fluctuations in the reconstruction order at length scales smaller than l_{rec}. In x-ray diffraction from such a growing interface, one would observe not only power law shaped peaks associated with the surface roughness, but also, at temperatures where l_{rec} is larger than the coherence length of the surface, power law shaped reconstruction diffraction peaks.

At length scales larger than l_{rec}, the surface appears as unreconstructed rough. Loops of that size are destroyed by nucleation of new loops instead of KPZ surface fluctuations, and they are not trapped anymore, because loop segments can hop across subvalleys of size $l>l_{\mathrm{rec}}$ by means of nucleation of new loops in subvalleys.

In our study we chose to focus on KPZ type surface growth dynamics, but we have good reasons to expect that the trapping of domain walls on ridge lines is a common phenomenon. In general, the quasicritical fluctuations will reflect the dynamic exponent of whatever growth dynamics is applicable. In recent studies of 1D models with KPZ and Ising type coupled degrees of freedom, the Ising defects became trapped in valleys and canyons and thus pinned down the growth [26,27]. We expect that a tendency toward faceting instead of ridge-line trapping can also be realized in our 2D model by varying the local growth rates.

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