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LETTER TO THE EDITOR

Interface growth with competing surface currents

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Abstract. We examine the dynamics of interface growth under the combined influence of a stabilizing and a destabilizing surface current in 1+1 dimensions. It has been shown that the surface is weakly stablized if a newly deposited particle can move locally to maximize the total number of nearest-neighbour contacts with the surface (curvature-driven current). The introduction of a weak, destabilizing surface tension term results in an almost periodic, grooved surface. The width of the surface grows linearly in time and does not reach a steady state. It appears that such a formation cannot be described by a continuous Langevin equation.

The evolution of growing surfaces has been extensively studied [1]. One of the basic questions that has been addressed is how the roughness of the surface depends on the dynamical rules of specific deposition processes. As a trivial example, the growth of independent columns without any local interactions produces a rough surface in which the width grows with the square root of time, so that a finite size system never reaches a steady state. When interactions between columns occur, a finite-size system can approach a steady state in the long-time limit [2–4]. For many classes of models, it has been well established that the time evolution of the width w is described by a scaling relation [5],

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

where L is the transverse linear dimension of the system, t is the time, and the scaling function f has the asymptotic behaviours $f(x) \sim x^{\beta}$, with $\beta = \zeta/z$, for $x \ll 1$, and $f(x) \sim$ constant for $x \gg 1$. Consequently the limiting behaviour of the width are

$$w \sim L^{z} \qquad t \gg L^{z} \tag{2a}$$

$$w \sim t^{\beta} \qquad t \ll L^{z}. \tag{2b}$$

An important example where intercolumn interactions lead to a steady state is the Edwards–Wilkinson (EW) model, where the surface current is driven by local height differences [6]. An incoming particle rolls down the surface from the initial contact point and is incorporated into the deposit upon reaching a local minimum. In the continuum limit, the dynamics of this rearrangement process can be described by the linear diffusion equation with a noise source,

$$\frac{\partial h(x,t)}{\partial t} = \mu \nabla^2 h(x,t) + \eta(x,t) \tag{3}$$

where $h(x, t)$ denotes the deviation of the height of the deposit from its average value

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at position x and time t, and $\eta(x, t)$ can be taken to be Gaussian random noise,

$$\langle \eta(x, t) \rangle = 0 \qquad \langle \eta(x, t)\eta(x', t') \rangle = \delta(x - x')\delta(t - t'). \tag{4}$$

The solution to (3) leads to a relatively smooth surface with roughness exponents $\zeta = \frac{1}{2}$ and $\beta = \frac{1}{4}$ in the $(1+1)$-dimensional case [6].

Recently, a different surface rearrangement mechanism has been investigated by Wolf and Villain [7] and Das Sarma and Tamborenea [8], in which the surface current is driven by local energy (i.e. curvature) differences. This mechanism may provide a useful description of molecular beam epitaxy growth. The curvature-driven (CD) current is modelled by allowing the newly added particle to move within a finite local region (for example, among lateral nearest neighours) to maximize the number of contacts—the 'valence'—between the particle and the original surface. This rearrangement leads to roughness exponents which are larger than those in the EW model. Simulations indicate that in $(1+1)$ dimensions the width follows (1) and (2), with $\zeta = 1.4 \pm 0.1$ and $z = 3.8 \pm 0.5$. For this model, it was also proposed [7, 8] that the continuum limit of the dynamics is described by the linear equation

$$\frac{\partial h(x, t)}{\partial t} = -\nu \nabla^4 h(x, t) + \eta(x, t) \tag{5}$$

whose solution yields $\zeta = \frac{3}{2}$ and $z = 4$, in good agreement with simulations.

This agreement is surprising, however, because the large surface roughness implied by $\zeta = \frac{3}{2}$ is inconsistent with the underlying small-gradient assumption of the continuum-equation description. A potential source of the inconsistency is the non-local nature of the current in the vertical direction at long times. Simulations reveal that the steady-state configuration in this model has many steep steps, indicative of the slope being an increasing function of the length scale. A particle which is added at a steep step therefore has to examine sites which are macroscopically distant vertically to find the site with the maximum number of contacts. This feature suggests that the curvature-driven model in its present form may not be adequate for describing the late stages of a real deposition process.

As an attempt to limit the non-locality of the vertical surface diffusion, we introduce a model in which a particle incident on a steep slope experiences a lateral attraction to the surface so that the particle can actually stick 'uphill' from its initial target point (figure 1(a)). We shall describe this feature in terms of a variable antigravity (or

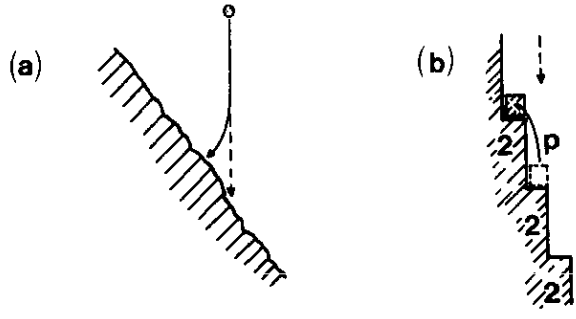

Figure 1. (a) Schematic illustration of the lateral attraction of an incident particle to the surface. (b) A microscopic realization of the upward current by the 'tie-breaking' when the valence in the 3-site neighbourhood, $v = (2, 2, 2)$. In this example a particle moves to the highest site with probability p.

negative surface-tension) current, and investigate the competing effects of the negative surface-tension and curvature-driven currents. To realize the negative surface tension microscopically, we intrdouce an additional repositioning criterion beyond that in the CD model, whenever the microscopic rules of the CD model permit more than one choice for the final particle position. Writing the valence in the three-site neighbourhood of i as $v=(v_{i-1}, v_i, v_{i+1})$, then, for example, no repositioning takes place in the microscopic model of [7] for $v=(2,2,1)$ or $v=(2,2,2)$, while the particle moves at random to a nearest neighbour when $v=(3,1,3)$. In our model, the 'tie' is resolved by imposing an additional rule which favours the attachment of the particle to the highest point in the local neighbourhood (figure 1(*b*)). This rule is opposite to the rearrangment process of the EW model, and gives rise to an infinitesimal destablization which competes with the stabilizing curvature-driven current.

For our competing current model, we simulated periodic systems with the linear dimension L in the range 2–1000, and followed the evolution of the surface for up to 2^{22} time steps. To control the strength of the negative surface tension, we introduce a parameter $0 \leq p \leq 1$, which gives the probability that in the case of ties in valence, the newly added particle actually sticks at the highest site in the neighbourhood, while with probability $(1-p)$ the particle chooses to stick at random among the neighbouring sites of the same valence (figure 1(*b*)). The original CD model corresponds approximately to the case $p=0$, while for $p=1$ there is maximal destablization. Figure 2 shows the form of the surface in the long time limit for various values of p.

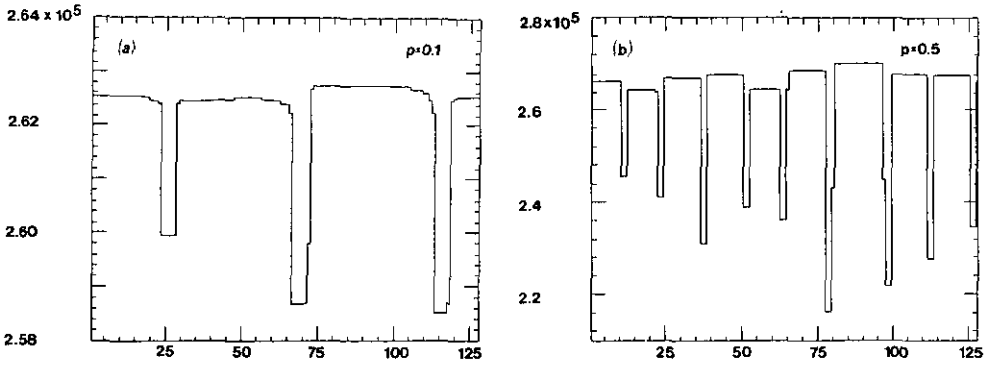

Figure 2. Steady state surface configurations for the competing-current deposition process for a system of linear dimension $L=128$ at 2^{18} time steps. Shown are the cases (*a*) $p=0.1$, and (*b*) $p=0.5$. In the latter case, the plateaux appear to be flat becuase of the large vertical scale.

Perhaps the most striking feature in these figures is the formation of a robust and almost periodic deeply grooved surface. There are two different macroscopic growth velocities for the plateaux and the grooves, so that the width of the surface grows linearly in time. The distance between grooves forms a nearly uniform distribution with the upper limit typically equal to twice the lower limit. For example, when $p=\frac{1}{2}$, the minimum distance between grooves is 11 and the maximum is 21. As p decreases, the groove separation and width both increase and ultimately diverge as $p \to 0$. When L is smaller than the minimum distance between grooves for a given value of p, then the surface grows in a stable manner, with the width saturating to fine value at long times. As a function of L, there is a transition line, $p=p_c(L)$, below which the surface reaches a steady state and above which a grooved surface occurs (figure 3). For fixed

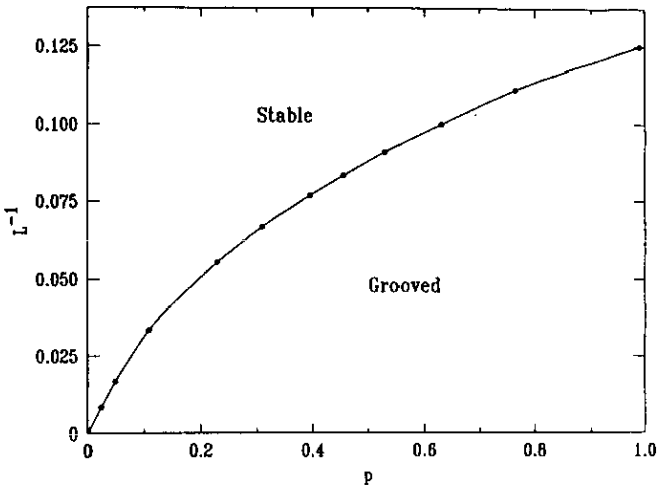

Figure 3. Phase diagram of the competing-current deposition process in the p–L^{-1} plane. The errors associated with the data points are smaller than the size of the point. The line is drawn as a guide to the eye only.

L, we determine the transition point by monitoring the time dependence of the width and looking for the value of p where the asymptotic behaviour crosses over from linear growth to saturation at a finite value. The accurate location of this transition point is time consuming due to the long relaxation time until the surface exhibits its asymptotic temporal behaviour. For a large system, the distance between grooves is proportional to the inverse function $L_c(p)$. Numerically, we find that this distance diverges as $p^{-\gamma}$ as $p \to 0$, with $\gamma = 0.9 \pm 0.1$.

We can give the following heuristic argument for the p dependence of the distance between grooves. For small p, the growing surface develops grooves only when the system is larger or equal to a critical size L_c. The formation of grooves at L_c is driven by the competition between the curvature-driven and negative surface tension-driven currents. In the $p \to 0$ limit, the surface consists primarily of consecutive steep steps, since the roughness exponent ζ exceeds unity. In the neighbourhood of these steps, the negative surface tension generates an upward current. Within the scale of a single groove, the net upward current is proportional to pL, which is the product of the upward hopping probability at the steps times the spatial extent of the steps. On the other hand, the curvature-driven term generates a current from the plateau into the groove, but this contribution occurs only at the edge of a plateau. Since there is typically of the order of one such location on the length scale of a single groove, the downward current is of order unity. At the boundary between grooved and stable growth, these two currents should balance. Thus we suggest that $L_c \sim p^{-1}$, i.e. $\gamma = 1$, consistent with our numerical estimate.

Further insights into the underlying mechanism for the groove instability can be obtained by considering small systems. Numerical simulations or our competing current model at $p = 1$ show that the surface is stable (no grooves) for linear dimension $L \leqslant 7$, but is unstable to the formation of a single deep groove for $L \geqslant 8$, in the long-time limit. To understand the mechanism responsible for this instability, we consider a growth model which possesses a stronger destabilizing current than in the competing current model, but still exhibits a groove instability of a similar nature. The transition

in the modified model occurs at a small enough value of L that we can provide an analytical description of the transition.

We realize the stronger destablizing current by the following augmentation to the surface rearrangement rules of the competing current model (figure 4). Qualitatively, this enhancement permits some degree of surface rearrangement by the simultaneous increase in the particle height and decrease in the number of nearest-neighbour surface contacts. When the valence at a neighbouring site j is larger than the valence at the incident site i by $+1$, the newly added particle remains fixed with probability α and moves with probability $1-\alpha$ if the move decreases the particle height ($\Delta h<0$), and always moves if the particle height remains the same. When the valence at neighbouring sites is the same as at the incident site, a lateral move occurs only if $\Delta h>0$. Finally, when the valence at j is smaller than the valence at i by -1, the newly added particle remains fixed with probability $1-\alpha$ and moves with probability α if $\Delta h>0$, and does not move if the particle height remains the same.

The case $\alpha=0$ corresponds to the competing current model with $p=1$, for which stable surface growth occurs for $L\leqslant 7$. However for $\alpha=1$, grooved surface growth occurs already when $L=3$. This can be understood by considering what happens when the first two particles are incident on adjacent sites. Due to the enhanced destabilizing current, the new particle is moved on top of the first particle. Thus independent of the location of incident particles, a single tower grows for $\alpha=1$. Since a smooth surface grows for $\alpha=0$, we expect a transition from stable to grooved surface growth as α is varied between 0 and 1. To locate this transition, we map the interface dynamics onto a random walk process whose individual steps reflect the various ways that a surface is modified upon the addition of a single particle. With periodic boundary conditions, a surface configuration for $L=3$ can be represented by $\boldsymbol{n}=(n_1, n_2)$, where $n_i=h_{i+1}-h_i$ is the height difference between sites i and $i+1$. The periodic boundary condition implies that $n_3=h_1-h_3=-n_1-n_2$. Deposition of a particle at i results in $n_{i-1}\rightarrow n_{i-1}+1$ and $n_i\rightarrow n_i-1$. Thus in the (n_1, n_2) plane, the addition of a particle at site i is equivalent to hopping from $\boldsymbol{n}$ to $\boldsymbol{n}+\boldsymbol{d}_i$, $i=1,2,3$, with $\boldsymbol{d}_1=(-1,0)$, $\boldsymbol{d}_2=(1,-1)$, and $\boldsymbol{d}_3=(0,1)$ (figure 5).

To determine the long-time properties of this random walk, it is sufficient to consider only the fourth quadrant $n_1>0$ and $n_2<0$. Permutations of the surface column heights correspond to the remaining quadrants. Define $P_i(\boldsymbol{n})$ as the probability of hopping from $\boldsymbol{n}$ to $\boldsymbol{n}+\boldsymbol{d}_i$. By enumerating the possible changes in the surface upon the addition of a single particle, we find $\boldsymbol{P}\equiv(P_1(\boldsymbol{n}), P_2(\boldsymbol{n}), P_3(\boldsymbol{n}))=(1-2\alpha/3, \alpha/3, \alpha/3)$ for $n_3<0$,

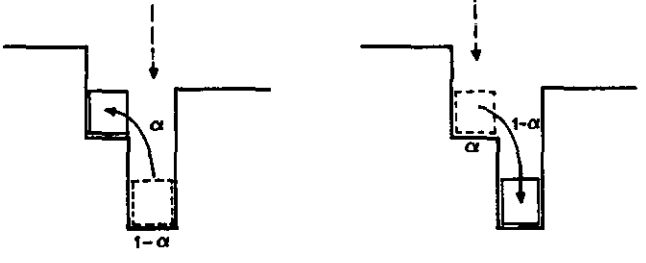

Figure 4. Illustration of the additional surface rearrangement processes that can occur when the negative surface tension term is enhanced by allowing an incident particle to move to a neighbouring site with a valence decreased by one, but with a larger height. Shown is an example involving a possible transition between sites of valence 2 and 3; a similar situation exists for two neighbouring sites with valence 1 and 2.

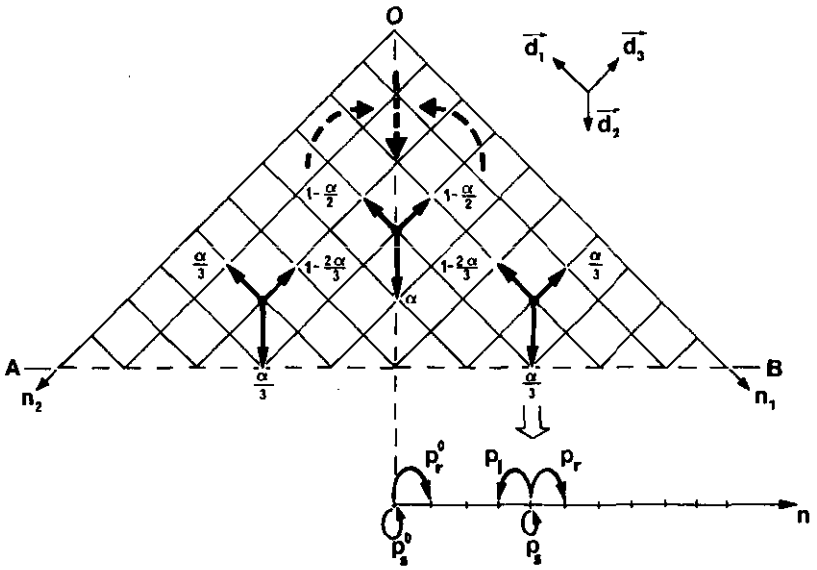

Figure 5. Equivalent random walk to describe the growth of a periodic 3-column surface according to the competing current model with enhanced negative surface tension. Shown are the step directions d_i which correspond to adding a single particle at site i (upper right). In the four quadrant of the n_1–n_2 plane, the hopping probabilities that correspond to adding a single particle at sites 1, 2, and 3, are indicated. The hopping probabilities projected onto the $\overline{QB}$ interval are also shown. The dashed arrows indicate the direction of the probability current on a broad scale for $\frac{1}{3}<\alpha<\frac{1}{2}$.

$\boldsymbol{P}=(\alpha/3,\ \alpha/3,\ 1-2\alpha/3)$ for $n_3>0$, and $\boldsymbol{P}=((1-\alpha)/2,\ \alpha,\ (1-\alpha)/2)$ for $n_3=0$. If the random walk approaches the origin at long times, it implies that the surface is smooth, while if the walk escapes to infinity, a surface with a deep groove is formed.

To solve this problem, we separately consider the random walk motion projected onto the horizontal line $\overline{AB}$ which is perpendicular to the $n_3=0$ axis, and the vertical motion (figure 5). To determine whether the random walk approached the origin in the long-time limit, we shall compute the average vertical current, averaged over the steady-state probability distribution along $\underline{B}$. Due to reflection symmetry with respect to the $n_3=0$ axis, the projected horizontal problem can be reduced to the half interval $\overline{QB}$, with a reflecting boundary condition at the symmetry point Q. For interior points, the hopping probability to the left (toward Q) is $p_l=1-2\alpha/3$, the hopping probability to the right is $p_r=\alpha/3$, and the probability of not hopping is $p_s=\alpha/3$. At Q, the probability of hopping to the right is $p_r^0=1-\alpha$ and the probability of not hopping is $p_s^0=\alpha$. Using conventional generating function methods, the horizontal steady-state probability distribution is $\mathcal{P}(m)=[3(1-\alpha)/2\alpha][\alpha/(3-2\alpha)]^m$ for $m=1, 2, 3, \ldots$ and $\mathcal{P}(0)=\frac{1}{2}$, where m is the distance from the boundary point Q. Here we have assumed an infinite half-interval, appropriate for $\overline{QB}$ far from the origin.

The vertical components of the hopping probabilities give rise to a net vertical current at horizontal position m which is given by $j(m\neq 0)=(1-\alpha)/2$ and $j(0)=(1-3\alpha)/2$. This leads to a mean steady-state curent $\langle j\rangle=\Sigma_m j(m)\mathcal{P}(m)=(1-2\alpha)/2$. Thus for $\alpha>\frac{1}{2}$, there is a net probability current toward infinity, indicative of grooved surface growth in the long-time limit, while for $\alpha<\frac{1}{2}$, the current flows to the origin, and smooth surface growth occurs. For larger system sizes, we expect that a similar approach will give a decreasing value of α at which grooved surface growth first appears.

Finally we discuss the possibility of a continuum-equation description for the competing-current growth model. Naively, one might expect that the competing currents could be described by a linear diffusion equation which contains a stabilizing quartic term and a destabilizing quadratic term. Such an equation selects a characteristic length scale, whose qualitative dependence on phenomenological parameters mirrors the p dependence of the distance between grooves in the competing current model. However in this continuum equation, there are a range of wavenumbers for which the surface is unstable. The linear equation also yields a different morphology than in the competing current model. Another possibility is that the competing current is described by a higher-order surface tension term [9], i.e. $-\lambda\nabla(\nabla h)^3$ and $\lambda > 0$. This is a relevant contribution with respect to the fourth-derivative term in (5), and serves to destabilize the surface. Numerical integration of the resulting equation leads to 'spiky' formations, but not of the qualitative form as the grooves in the competing current model. Furthermore, since the two driving terms in the continuum equation involve the same power of spatial derivatives, a characteristic length scale is not selected, in contrast to our discrete model. Thus it appears that a simple continuum equation cannot describe the existence of a phase in which the surface exhibits a quasi-periodic array of grooves.

In conclusion, we introduced a new model which includes a destabilizing negative surface-tension current (antigravity) in addition to a stabilizing curvature-driven current. The stability of the surface with respect to this destabilizing current was examined. The resulting surface exhibits a robust instability in which a nearly periodic array of grooves is formed. The wavelength of this periodicity can be controlled by tuning the strength of the destabilizing surface current. In the grooved phase, the surface width increases linearly in time and there is no steady state. Up to fourth-order terms in spatial derivatives, a continuous Langevin equation is inadequate to describe the surface morphology that arises from this competing current growth mechanism.

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References

[1] Krug J and Spohn H 1990 *Solids Far From Equilibrium: Growth, Morphology, and Defects* ed C Godriche (Cambridge: Cambridge University Press)
Family F 1990 *Physica* **168**A 561
[2] Kardar M, Parisi G and Zhang Y-C 1986 *Phys. Rev. Lett.* **56** 889
[3] Kim J M and Kosterlitz J M 1989 *Phys. Rev. Lett.* **62** 2289
[4] Kerterz J and Wolf D E 1989 *Phys. Rev. Lett.* **62** 2571
[5] Family F and Vicsek T 1985 *J. Phys. A: Math. Gen.* **18** L75
[6] Edwards S F and Wilkinson D 1982 *Proc. R. Soc.* A **381** 17
[7] Wolf D E and Villain J 1990 *Europhys. Lett.* **13** 389
[8] Das Sarma S and Tamborenea P 1991 *Phys. Rev. Lett.* **66** 325
[9] Lai Z-W and Das Sarma S 1991 *Phys. Rev. Lett.* **66** 2348
Villain J 1991 *J. Physique I* **1** 19