Linear growth equation with spatiotemporally correlated noise to describe the meandering instability

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Abstract: We present analytical and kinetic Monte Carlo simulation (KMC) study for the (2+1) dimensional discrete growth model. A non-local, phenomenological continuum equation describing surface growth in unstable systems with anomalous scaling is proposed. The roughness of the unstable surface, originated from an Ehrlich-Schwoebel (ES) barrier, is then studied under various deposition fluxes. The induced meandering instability is found, unexpectedly, to be described by a linear growth continuum equation but with spatiotemporally correlated noise.

1. Introduction
The discovery of scale invariance in systems out of equilibrium has opened up several exciting investigation fields in the last 20 years [1]. One of these is concerned with the scaling properties of kinetic roughening of growing crystal surfaces [2]. Partly motivated by Molecular Beam Epitaxy (MBE), which allows investigation of growth processes at the atomistic level, and is a crystal growth technique of considerable technological relevance, the comprehension of this phenomenon is important for the understanding and control of the surface morphology and nanostructures. Both numerical simulations and experiments have observed that a large variety of growth processes can be divided into only a few universality classes [2,3].

Each class is characterized by the specific values of the two scaling exponents: the roughness exponent \( \alpha \) and the growth exponent \( \beta \). Specifically, with \( h(r,t) \) denoting the surface height (relative to an initial vicinal plane of reference) at position \( r \) and time \( t \) starting from a perfect vicinal substrate, the height-height correlation function defined by: 

\[
G(r,t) = \overline{[h(x+r,t) - h(x,t)]^2}
\]

(here, the overbar denotes spatial average and the angular brackets denote statistical ensemble-average), satisfies the dynamic scaling ansatz [3]:

\[
G(r,t) = t^{2\beta} g(r/\xi), \tag{1}
\]

where the scaling function \( g(u) \sim u^{2\alpha} \) for \( u \ll 1 \) and \( g(u) \sim \text{constant} \) for \( u \gg 1 \). We consider the case of (2+1)D surface where \( \xi \sim t^{1/2} \) is the correlation length, and dynamic exponent \( z = \alpha / \beta \).

The important features of growing surfaces can usually be analyzed and described by some microscopic rules. A number of discrete models for growth phenomena have been proposed and
studied successfully by computer simulations. On the other hand, evolution of the growing surface is also, in the coarse-grained sense, described by a continuum equation with additive noise [2,3]. It is generally believed that there is a correspondence between discrete growth models and continuous stochastic Langevin equations. The most common way of establishing the link is to compare the values obtained for scaling exponents. Another way is to derive the continuum equation from a given discrete model analytically [4,5]. However, in order to approach real experimental morphology, numerical discrete models must include some atomistic mechanisms, such as Ehrlich-Schwöbel (ES) barriers (well known for explaining unstable growth in MBE), which is believed to be described by non linear continuum equation [6,7]. In this case, the main difficulty is to resolve the continuum equation analytically.

Most frequently the grown surface in fact develops kinetic instability or regular spontaneous structures, which imply that interface correlations play an essential role in determining the final surface morphology. Therefore, beyond the numerical results, it is important to understand the physical origin of these correlations. We believe that interface structure is closely linked to the surface correlation shape and its strength. Actually, after Villain’s demonstration of the non-equilibrium current [6] responsible for unstable growth (meandering instability), it is common to describe the interface correlations with a non-linear term plus an uncorrelated white noise. Here, on the basis of an SOS (Solid on Solid) simulation model of unstable vicinal surface, we propose a phenomenological description of these correlations using a continuum equation, but with space-time correlated noise. In fact, the main idea is to include the interface spatiotemporal correlations in the noise term and interpret it as a phenomenon induced by the instability itself and also by matter-transport. Recently, a space-time correlated noise was proposed by Pang et al. [8] to describe the super-roughening using a linear growth equation in (1+1) dimensions:

\[
\frac{\partial}{\partial t} h(x,t) = (-1)^{m+1} \nabla^{2m} h(x,t) + \eta(x,t),
\]

\[
<\eta(x,t)\eta(x',t')> = D|x-x'|^{2\rho-1}|t-t'|^{2\theta-1}, \text{ with } 0 \leq \rho, \theta < 1/2,
\]

where \( \eta(x,t) \) represents a Gaussian-distributed noise of zero mean and power-law spatiotemporally-decaying correlation. Its initial variant is spatial and temporal correlation, proposed by Yi-Kuo and Pang to study the EW model [9]. Note that, for \( m=1 \) and \( m=2 \), the last equation with white noise denotes respectively the well-known Edwards-Wilkinson equation [9] and the Mullins-Wolf-Villain equation [10]. By using simple scaling analysis, it is straightforward to obtain the following analytical expressions of the global roughness exponent \( \alpha \) and the dynamic exponent \( z \):

\[
\alpha = \phi + (2m - 1)/2, \quad z = 2m, \text{ with } \phi = 2m\theta + \rho.
\]

We note that \( z \) is independent of the noise shape (\( \rho \) and \( \theta \)) and that \( \alpha > 1 \). Thus, the interfacial growth processes described by equations (1) and (2) display super-roughening phenomena.

In this work, we used the form of this noise, characterised by a correlation parameter \( \phi \), to interpret our numerical scaling exponents deduced from a (2+1)D vicinal surface.

2. Roughening and meandering instability

After the introduction of conserved-particle surface diffusion equation for MBE realistic microscopic models three decades ago (in the 90s), such as the Wolf-Villain equation (WV) [10], as well as its non linear variant due to Villain [6], Lai and Das Sarma [7], the relaxation is governed by a Laplacian squared (non-linear) term, arising from a quasi-equilibrium contribution to the surface diffusion current. These authors show that the intrinsically nonequilibrium conditions yield surface diffusion processes that a tilt-dependent mass current, ultimately responsible for the scaling properties of these models. In particular, if the nonequilibrium contribution to the net diffusion current is a decreasing function of the inclination, it stabilizes the surface, leading generically, but somewhat surprisingly, to dynamic scaling characteristic of the linear Edwards-Wilkinson universality class [2]. By contrast, a non-equilibrium surface diffusion current yields a growth instability, resulting in a grooved state. The aim of this section is to better describe the kinetic roughness character induced by the meandering instability. Here, we propose a higher order EW-like equation to describe the scaling properties of our unstable growth model. For that reason, we studied the scaling properties of a destabilized surface by
an Ehrlich-Schwoebel (ES) barrier. The growth temperature is now fixed at $T=700K$ and the ES barrier is $E_b=0.1eV$. Figure 1, shows the images of the surface morphology with increasing flux: $F=1, 5, 20, 40$ ML/s. Three features could be distinguished: at relatively low flux, $F=1$ ML/s, deep grooves develop characteristic of the meandering instability induced by a strong ES effect. At higher deposition flux, knolls are well established (a hill-shaped structure is well established). Indeed, at intermediate temperature, $F=5$ ML/s, hillocks develop on the meanderings leading to crossover between the two last structures. The mean meander (or hill) size determines the correlation length $\xi$.

The critical exponents measured in the kinetic roughness regime, after deposition of 1000 ML, were reported in table bellow.

Table 1. Scaling exponents versus deposition flux $F$ (ML/s).

| $F$ (ML/s) | 1  | 5  | 20 | 40 |
|-----------|----|----|----|----|
| $\alpha_{loc}$ | 0.87 | 0.85 | 0.81 | 0.78 |
| $\beta$ | 0.72 | 0.62 | 0.54 | 0.51 |
| $\gamma$ | 5.88 | 5.91 | 6.02 | 6.02 |
| $\alpha=\beta$ | 4.23 | 3.65 | 3.25 | 3.07 |
| $\kappa \equiv \beta-\alpha_{loc}/\gamma$ | 0.57 | 0.48 | 0.40 | 0.38 |
| $\kappa$ | 0.62 | 0.48 | 0.39 | 0.38 |

Figure 1. Monte Carlo simulation images of the evolution of the surface morphology with increasing flux: $F=1, 5, 20, 40$ ML/s. The initial surface is a vicinal $(800\times800)$ sites (expressed in lattice unit) with terrace width $L=5$ sites.

From table 1 we can see that all critical exponents decrease as flux increases, except that the dynamic exponent $\gamma$ is fairly constant. Now, from our numerical scaling exponents, we will try to construct a phenomenological continuum equation describing the kinetic roughness of these unstable surfaces. The previous discussion about continuous equations suggested in the literature shows us that only one equation could be candidate to provide this modelling: the equation of Pang et al. (equation (2)). Indeed, all equations including nonlinear terms, like KPZ or LDV, lead to scaling relations, typically with: $\alpha+\gamma=\text{const}$, which implies that $\alpha$ cannot vary independently of $\gamma$. However, in our simulations with the ES effect, note that this last exponent is nearly constant versus flux, while $\alpha$ undergoes noticeable variation. The Pang equation, being linear, implies that, while $\alpha$ is a function of the parameters describing the correlation shape through $(\rho,\theta)$. This last point is particularly interesting. Indeed, the meandering instability, induced by an ES barrier, has a diffusive origin [11]. Kinetic roughness is due to fluctuations (noise) in the deposition flux, but it is coupled with unstable morphology thanks to diffusive transport. This gives rise to the space-time correlations in the noise (equation (3)) introduced into equation (2). Thus, we are tempted to propose the following equation to describe anomalous multi-affine kinetic roughness of an unstable vicinal surface:

\[
\frac{\partial}{\partial t} h(x,t) = -\nu \frac{\partial^6}{\partial x^6} h(x,t) + \eta(x,t),
\]

with $\eta(x,t) = 0$, and $\eta(x,t)\eta(x',t') = D|x-x'|^{2\rho-1} |t-t'|^{2\theta-1}$. (23)

We easily deduce: $0 \leq \rho, \theta < 1/2$, $0 \leq \phi = \rho+6\theta < 5/2$. A vanishing correlation parameter, $\phi=0$, corresponds to uncorrelated noise (white noise); at the other limit, $\phi = 5/2$ corresponds to maximum correlation.

The critical exponents expressed with the noise parameter, $\phi$, reads:
\[ \alpha = \phi + 5/2, \quad z = 6, \quad \beta = (\phi + 5/2)/6 \quad \text{and} \quad \kappa = (\phi + 3/2)/6, \quad \text{where} \quad \phi = 6\theta + \rho, \]

For example, if \( \phi = 2 \), we obtain:

\[ \alpha = 9/2 = 4.5, \quad z = 6, \quad \beta = \alpha/z = 3/4 = 0.75 \quad \text{and} \quad \kappa = (\alpha - 1)/z = 7/12 \approx 0.58. \]

These later values are to be compared to our simulation exponents \((\alpha_z, \beta, \kappa) = (4.23, 5.9, 0.72, 0.62)\) at a flux: \( F = 1 \) ML/s and fixed temperature \( T = 700K \). In a more general way, one can easily check that \( \beta \) and \( \kappa \) exponents must vary linearly with \( \alpha \). Plotting \( \beta \) and \( \kappa \) versus \((\alpha - 5/2)\), we expect:

\[ \beta = (\alpha - 5/2)/6 + 5/12, \quad \text{and} \quad \kappa = (\alpha - 5/2)/6 + 3/12. \]

Figure 2, shows the plot of equation (9), the linear fit reads:

\[ \beta = 0.18(\alpha - 5/2) + 0.41, \quad \kappa = 0.166(\alpha - 5/2) + 0.28, \]

equation (27) is in good agreement with the theoretical prediction (eqn. (8)).

Our argument implies that, a growing flux leads to a decreasing trend in surface diffusion. Consequently, it involves less correlations in the morphology, and thus in the noise. Therefore, we expect that an increase in the deposition flux, causes a reduction of the correlation range in the noise through \( \phi \).

Using the numerical simulation data of critical exponents, realised for various deposition flux \( F \), we determine an interesting relation between the noise feature, \( \phi_{\text{sim}} \), and \( F \):

\[ \phi_{\text{sim}} = (\alpha_{\text{sim}} - 5/2) \approx 2.1F^{-0.28 \pm 0.01}. \]

One expects that the parameter which controls the meandering instability to be the ratio:

\[ (c_{eq}D/F)^{\gamma}, \]

where \( c_{eq} = \exp(-2E_d/k_BT) \). Using \( E_d = 1.0 \) eV and \( E_a = 0.3 \) eV, then at \( T = 700K \), we compute:

\[ c_{eq}D = \frac{10^{13}}{2}\exp\left( -\frac{E_d}{k_BT} \right) = 15.03. \]

If we use \( \gamma = 0.28 \), it follows:

\[ (c_{eq}D/F)^{0.28} = 2.13F^{-0.28}. \]

Thus, the former result (eqn. (12)) lends more credibility to our initial assumption: the correlations in the noise are induced by the meandering instability and mediated by surface diffusion.
3. Conclusion
Assuming that the correlations in the meandering instability are included and described by the noise-shape, we have proposed a phenomenological continuum equation for the space-time correlations between the close-sites and then solved analytically. Our Monte-Carlo atomistic model, exhibits kinetic roughening due to limited interface diffusion and unstable growth leading to a self-organised pattern with deep grooves, then to mounding originating from the Ehrlich-Schwoebel barrier near step edges. The data obtained analytically were found to be in a good agreement with our growth-model numerical results and even allows an explanation to be given for the correlation of the noise such as a phenomenon induced by the instability itself and the matter-transport. The meandering instability induced by an ES effect, seems to be well described by a linear continuous equation with spatiotemporally correlated noise. This appears incompatible with the nonlinear character of the smoothing term induced by the instability. However, the latter term does not appear explicitly in the growth equation, whereas it is included implicitly in the noise whose form was proposed by Pang et al. [8].

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References
[1] G. Odor, *Rev. Mod. Phys.* **76**, (2004) p663.
[2] A.-L. Barabasi and H. E. Stanley, *Fractal Concepts in Surface Growth* (Cambridge University Press, Cambridge, 1998).
[3] D. D. Vvedensky, A. Zangwill, C. N. Luse, and M. R. Wilby, *Phys. Rev. E* **48**, (1993) p852.
[4] Villain J., *Journal de Physique I* **1**, (1991) p19.
[5] Z.-W Lai. and S. Das Sarma, *Phy. Rev. Lett.* **66**, (1991) p2348.
[6] Pang Ning-Ning, Wen-Jer Tzeng, *Phys. Rev. E* **70**, (2004) 011105.
[7] S.F. Edwards and D.R. Wilkinson, *Proc. R. Soc. London, Ser. A* **381**, (1982) p17.
[8] D.E. Wolf and J. Villain, *J. Europhys. Lett.* **13**, (1990) p1350.
[9] G.S. Bales and A. Zangwill, *Phys. Rev. B* **41**, (1990) p5500.