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LETTER TO THE EDITOR

Conserved growth on vicinal surfaces

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Abstract. A crystal surface which is miscut with respect to a high-symmetry plane exhibits steps with a characteristic distance. It is argued that the continuum description of growth on such a surface, when desorption can be neglected, is given by the anisotropic version of the conserved KPZ equation with non-conserved noise. A one-loop dynamical renormalization group calculation yields the values of the dynamical exponent and the roughness exponent which are shown to be the same as in the isotropic case. The results presented here should particularly apply to growth under conditions which are typical for molecular beam epitaxy.

The fabrication of novel electronic devices requires experimental conditions which are highly controllable. Molecular beam epitaxy (MBE) is a very valuable technology for this purpose. In this process particles are deposited under high-vacuum conditions onto a crystal surface which has usually been cleaved prior to growth. The cleavage process may generate a surface which is miscut against a high-symmetry plane and which exhibits terraces with a characteristic width. The terrace size can be made very large, but a small miscut can never be avoided. Therefore the surface at the beginning of the growth process must always be regarded as *vicinal*.

Since desorption of adatoms can be neglected under experimental conditions which are typical for MBE, surface relaxation by adatom diffusion is volume conserving. This paper introduces the continuum description of such *conserved* growth on a vicinal surface. This allows for the analysis of the stochastic fluctations of the surface, which appear on large length and timescales during growth. The surface fluctuations, apart from being of interest in their own right, may be intimately related to the damping of oscillations observed during layer-by-layer growth, as has been shown recently [1, 2].

The surface fluctuations are expected to exhibit self-affine scaling [3]:

$$w(t) \simeq a_\perp(\xi(t)/\tilde{\ell})^\zeta \qquad \text{and} \qquad \xi(t) \simeq \tilde{\ell}(t/\tilde{t})^{1/z} \tag{1}$$

if the surface is isotropic. Here w is the root-mean-square variation of the film thickness (the surface width), $a_\perp$ is the thickness of one atomic layer, and ξ is the correlation length up to which the surface roughness has fully developed until time t. ζ is the roughness exponent and z the dynamical exponent. The layer coherence length $\tilde{\ell}$ and the oscillation damping time $\tilde{t}$ [1] play the roles of natural cut-offs in the continuum description of the surface fluctuations at small length and timescales. To calculate the values of z and ζ, we derive the equation governing conserved growth on vicinal surfaces next.

On a coarse-grained scale the surface can be described at any given time t by a single-valued function $h(x_\parallel, x_\perp, t)$. The coordinate system is chosen such that the surface tilt is m in the $x_\parallel$-direction, while the steps are along the $x_\perp$-direction. It is then convenient to work

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in a tilted coordinate system, $h \to h - mx_\parallel$, so that h represents the surface fluctuations around the average tilt. Since we consider conserved growth, the evolution equation for the surface has the form

$$\partial_t h = -\nabla \cdot \boldsymbol{j} + \eta + \mathcal{F} \tag{2}$$

with a surface diffusion current $\boldsymbol{j}$ and a noise term η which models the disorder entering the mesoscopic description (2) due to the stochastic nature of the growth process. With the abbreviations $\partial_\parallel \equiv \partial/\partial x_\parallel$ and $\partial_\perp \equiv \partial/\partial x_\perp$, the vector ∇ reads $(\partial_\parallel, \partial_\perp)$. $\mathcal{F}$ is the average particle flux which is formally eliminated by changing to the comoving frame, $h \to h - \mathcal{F}t$. All lattice constants are set to unity for convenience.

The surface diffusion current has an equilibrium contribution and a non-equilibrium contribution, $\boldsymbol{j} = \boldsymbol{j}_{\rm eq} + \boldsymbol{j}_{\rm neq}$. $\boldsymbol{j}_{\rm eq}$ is given by the tendency of the adatom current to even out gradients in the local equilibrium chemical potential $n_{\rm eq}$ of the surface, $\boldsymbol{j}_{\rm eq} = -\Gamma \nabla n_{\rm eq}$. Γ is the adatom mobility, which for simplicity is assumed to be isotropic. $n_{\rm eq}$ depends on h like

$$n_{\rm eq} = -\left(\frac{\kappa_\parallel}{\Gamma}\partial_\parallel^2 + \frac{\kappa_\perp}{\Gamma}\partial_\perp^2\right) h. \tag{3}$$

$\kappa_\parallel/\Gamma$ and $\kappa_\perp/\Gamma$ are the anisotropic surface stiffnesses [4–6], which for small variations of the surface can be regarded as constant. Equation (3) represents the Gibbs–Thomson effect.

The non-equilibrium contribution $\boldsymbol{j}_{\rm neq} = -D\nabla n_{\rm neq}$ to the surface current is driven by the non-equilibrium adatom density $n_{\rm neq}$ [7]. D is the (isotropic) diffusion constant. On a flat surface without steps, n_0 is of the order of $(F/D)\ell_D^2$, as derived in [8]. ℓ_D denotes the typical island distance on a flat surface [9]. We assume ℓ_D to be isotropic, which is the case if diffusion and lateral bonding of adatoms to islands is isotropic. When steps are present and the tilt is strong enough to suppress island nucleation on terraces, i.e. if $|m|\ell_D \gtrsim 1$, n_0 depends on the local surface tilt: $n_0 \propto (\mathcal{F}/D)/|m|^2$. A convenient ansatz for interpolation between those two regimes is [10]

$$n_{\rm neq}(\nabla h) = \frac{n_0}{1 + \ell_D^2[(m + \partial_\parallel h)^2 + (\partial_\perp h)^2]} \tag{4}$$

in our coordinate system. $n_{\rm neq}$ can be expanded for small deviations from the global tilt to give

$$n_{\rm neq}(\nabla h) \simeq n_{\rm neq}(0) - \frac{\mu_\parallel}{D}\partial_\parallel h - \frac{\lambda_\parallel}{D}(\partial_\parallel h)^2 - \frac{\lambda_\perp}{D}(\partial_\perp h)^2 \tag{5}$$

with the quantities $n_{\rm neq}(0)$, $\mu_\parallel$, and $\lambda_\perp$ being positive functions of $|m|$, n_0, and ℓ_D. For small tilts, $|m|\ell_D \lesssim 1$, $\lambda_\parallel$ is positive, while for large tilts, $|m|\ell_D \gtrsim 1$, it is negative. These two cases distinguish between nucleation-dominated growth and step-flow growth, respectively. The different signs of the nonlinearities are known to have dramatic consequences on the surface fluctuations in the case of non-conserved growth on vicinal surfaces, which is described by the anisotropic KPZ equation [11]. One aim of this study is to see if a similar scenario can be found in the conserved case.

The noise η has three contributions in MBE growth [9]: shot noise, diffusion noise, and nucleation noise. Shot noise arises due to statistical fluctuations in the atom beam which can be assumed to be isotropic. Diffusion noise has its origin in the stochastic motion of adatoms. Since we assume diffusion to be isotropic, this contribution is also isotropic. Finally, nucleation noise describes the random distribution of island nucleation locations. Because diffusion noise and shot noise together generate nucleation noise, the latter is also isotropic. In [12] it has been shown that nucleation noise is long-range correlated in time as long as the surface grows layerwise. The continuum approach we pursue here is applicable for times larger than the oscillation damping time, which marks the transition

from layer-by-layer growth to rough growth. After this time, the temporal correlations have ceased. Therefore we can assume nucleation noise to be short-range correlated in time for the present purpose. Note also that despite their relation on the microscopic level, there are no correlations between the different kinds of noise. With these remarks, the noise correlator reads [9, 13]

$$\langle \eta(x,t)\eta(y,s)\rangle = [\mathcal{F} - \mathcal{D}\nabla^2 + \mathcal{N}(\nabla^2)^2]\delta^2(x-y)\delta(t-s) \tag{6}$$

where $\mathcal{F}$, $\mathcal{D}$, and $\mathcal{N}$ denote the strengths of the shot noise, the diffusion noise, and the nucleation noise, respectively. The average value $\langle\eta\rangle$ vanishes.

In summary, we arrive at the anisotropic conserved KPZ (ACKPZ) equation

$$\partial_t h = -\nabla^2[(\kappa_\parallel \partial_\parallel^2 + \kappa_\perp \partial_\perp^2)h + \mu\partial_\parallel h + \lambda_\parallel(\partial_\parallel h)^2 + \lambda_\perp(\partial_\perp h)^2] + \eta \tag{7}$$

where the noise correlator is given by equation (6). Note that the linear term proportional to μ cannot be transformed away as in the non-conserved case [11]. This equation with $\mu = 0$ was first studied in [14]. However, as the following analysis shows, the conclusion presented there has to be corrected. We study the surface fluctuations predicted by equation (7) next.

In the linear case $\lambda_\parallel = \lambda_\perp = 0$, equation (7) can be solved directly. One result is that the term $\propto \mu$ does not influence the surface fluctuations. Setting $\mu = 0$, we may obtain the values of the exponents by rescaling

$$x_\perp \to b x_\perp \qquad x_\parallel \to b^\chi x_\parallel \qquad t \to b^z t \qquad h \to b^\zeta h \tag{8}$$

where b is an arbitrary scaling factor [15]. The anisotropy exponent χ [11, 16] has to be introduced here to account for the fact that in contrast to equation (1), which is isotropic, there may be different characteristic lengths $\xi_\parallel$ and $\xi_\perp$ governing the morphology of the surface. χ is defined by the relation $\xi_\parallel \propto \xi_\perp^\chi$. By writing $b = \exp(\mathrm{d}\ell)$ with infintesimal $\mathrm{d}\ell$, we obtain

$$\frac{\mathrm{d}\kappa_\parallel}{\mathrm{d}\ell} = \kappa_\parallel(z - 4\chi) \tag{9}$$

$$\frac{\mathrm{d}r_\kappa}{\mathrm{d}\ell} = 4r_\kappa(1-\chi) \tag{10}$$

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}\ell} = \mathcal{F}(z - 2\zeta - 2) \tag{11}$$

$$\frac{\mathrm{d}\mathcal{D}}{\mathrm{d}\ell} = \mathcal{D}(z - 2\zeta - 4) \tag{12}$$

$$\frac{\mathrm{d}\mathcal{N}}{\mathrm{d}\ell} = \mathcal{N}(z - 2\zeta - 6) \tag{13}$$

for the change of the parameters in the continuum equation upon rescaling, where $r_\kappa \equiv \kappa_\parallel/\kappa_\perp$. From equations (11)–(13) we see that shot noise is the most relevant type of noise, since it grows the fastest upon an increase of scale for any values of z and ζ. For this reason we have to use equation (11) in the determination of the exponents. Requiring scale invariance of the surface amounts to setting the left-hand sides of the above equations to zero. Using equations (9)–(11), we find the exponents

$$z = 4 \qquad \zeta = 1 \qquad \chi = 1. \tag{14}$$

This means that a growing surface described by the linear version of equation (7) can only be scale-invariant if the two spatial coordinates are rescaled with the same scaling factor b. Then, the surface fluctuations are governed by the isotropic version of equation (7) with $\lambda_\parallel = 0$ and $\lambda_\perp = 0$.

The full (nonlinear) equation (7) is dealt with along the lines described in [15, 17]. Wavenumbers $b\pi/a \leqslant |k_\perp| \leqslant \pi/a$ and $b^\chi\pi/a \leqslant |k_\parallel| \leqslant \pi/a$, where a is the lattice constant

parallel to the surface, are integrated out (a is set to 1 for convenience). This is done in a one-loop approximation published in detail elsewhere [18]. The resulting renormalized parameters are then rescaled according to equation (8). It turns out that $\mathcal{F}$, $\lambda_\parallel$, and $\lambda_\perp$ are not renormalized. The corresponding flow equations are

$$\frac{\mathrm{d}\lambda_\parallel}{\mathrm{d}\ell} = \lambda_\parallel(z - 4\chi + \zeta) \tag{15}$$

$$\frac{\mathrm{d}r_\lambda}{\mathrm{d}\ell} = r_\lambda(1 - \chi) \tag{16}$$

and equation (11), where $r_\lambda \equiv \lambda_\parallel/\lambda_\perp$. Those three equations already fix the exponents to be

$$z = \tfrac{10}{3} \qquad \text{and} \qquad \zeta = \tfrac{2}{3} \tag{17}$$

if the system is scale invariant *and* if $\lambda_\parallel, \lambda_\perp \neq 0$. These are the values for the isotropic conserved KPZ equation in $d = 2$ [19, 13, 20] in one-loop order. (In two-loop order they are slightly modified [21].)

The one-loop corrections to the parameters do not depend on μ [18]. Thus, the corresponding term does not play a role in the determination of the surface fluctuations—as in the linear case. (Interestingly this does not hold for a related deterministic nonlinear equation which exhibits deterministic chaos [22].) For this reason, we set $\mu = 0$ in the following.

A remark on the noise renormalization is in order. The nucleation noise *is* renormalized and the corresponding flow equation reads

$$\frac{\mathrm{d}\mathcal{N}}{\mathrm{d}\ell} = \mathcal{N}[z - 2\zeta - 6] + g_\perp f(\kappa_\parallel, \kappa_\perp, \lambda_\parallel, \lambda_\perp, \mathcal{F}, \mathcal{D}, \mathcal{N}) \tag{18}$$

with $g_\perp \equiv (2\pi)^{-2}\mathcal{F}\lambda_\perp^2/\kappa_\perp^3$. f is non-negative for non-negative $\mathcal{F}$ or $\mathcal{D}$ [18]. This means that, even if nucleation noise was absent ($\mathcal{N} = 0$) initially, this type of noise would automatically be generated by deposition and diffusion noise—which is immediately clear in the microscopic picture. As mentioned above, however, we utilize equation (11) for the determination of the exponents.

$\kappa_\parallel$ and $\kappa_\perp$ also are renormalized. This can be discussed most conveniently by considering the flow equations for r_κ and $g_\perp$:

$$\frac{\mathrm{d}r_\kappa}{\mathrm{d}\ell} = \frac{g_\perp\pi}{4r_\kappa^{3/2}(r_\kappa - 1)^2}[9(r_\lambda^2 - r_\kappa^4) + r_\kappa^3(26 - 8r_\lambda) + r_\kappa r_\lambda(8 - 26r_\lambda) + 16(r_\lambda - 1)(r_\kappa^{5/2} + r_\kappa^{3/2}r_\lambda) + r_\kappa^2(r_\lambda^2 - 1)] \tag{19}$$

$$\frac{\mathrm{d}g_\perp}{\mathrm{d}\ell} = g_\perp\left[2 - \frac{3}{4}g_\perp\pi\,\frac{9r_\kappa^3 + r_\kappa^2(7r_\lambda - 26) - 16r_\kappa^{3/2}(r_\lambda - 1) + r_\kappa(10r_\lambda + 1) - r_\lambda}{r_\kappa^{3/2}(r_\kappa - 1)^2}\right]. \tag{20}$$

Note that in the limit of $r_\lambda, r_\kappa \to 1$, these flow equations reduce to the isotropic case as obtained in [19, 13]. Now the only important feature of these equations is whether the fixed point $g_\perp^* = 0$ is stable. If so, the nonlinearities would vanish on large scales and the growth exponents would take the values (14) given by the linear equation. This scenario is found for the anisotropic KPZ equation [11]. Here we wish to find out if the ACKPZ equation shows the same behaviour.

For fixed r_κ, it is clear from equation (20) that $g_\perp^* = 0$ is unstable, since $\mathrm{d}g_\perp/\mathrm{d}\ell = 2g_\perp$ for small $g_\perp$. Since equations (19) and (20) are coupled, however, $g_\perp^* = 0$ could in principle be reached for $r_\lambda < 0$ if r_κ vanishes together with $g_\perp$ in a suitable way, see equation (20). To see if this is possible, we consider the limit $r_\kappa \to 0$ of (19) and (20),

$$\frac{\mathrm{d}r_\kappa}{\mathrm{d}\ell} = \frac{9\pi g_\perp r_\lambda^2}{4r_\kappa^{3/2}} \tag{21}$$

$$\frac{\mathrm{d}g_\perp}{\mathrm{d}\ell} = g_\perp \left[2 + \frac{3\pi g_\perp r_\lambda}{4 r_\kappa^{3/2}} \right]. \tag{22}$$

To simplify the notation we set $r_\lambda = -8/(3\pi)$. For an initial condition $g_\perp > r_\kappa^{3/2}$, the coupling constant $g_\perp$ will initially decrease, see equation (22). For this decrease to continue, $g_\perp / r_\kappa^{3/2} > 1$ has to hold. Equation (21) then shows that r_κ, and consequently $g_\perp$, will increase again. Consequently, the fixed point $g_\perp^* = 0$ is always unstable. Thus, we can summarize that a change of universality class from the nonlinear to linear equation is not possible.

Therefore, in this paper it has been argued that the ACKPZ equation describes the fluctuations of a vicinal surface growing under MBE conditions. The dynamical and the roughness exponents are those of the isotropic conserved KPZ equation. In particular, the change from the nonlinear to linear universality class, as observed for the anisotropic KPZ equation [11], is not found here. Corroboration of these findings in experiments or computer simulations are left for future research.

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