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LETTER TO THE EDITOR

Coarsening in surface growth models without slope selection*

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Abstract. We study conserved models of crystal growth in one dimension ($\partial_t z(x,t) = -\partial_x j(x,t)$) which are linearly unstable and develop a mound structure whose typical size L increases in time ($L \sim t^n$). If the local slope ($m = \partial_x z$) increases indefinitely, n depends on the exponent γ characterizing the large-m behaviour of the surface current j ($j \sim 1/|m|^\gamma$): $n = \frac{1}{4}$ for $1 \leqslant \gamma \leqslant 3$ and $n = (1+\gamma)/(1+5\gamma)$ for $\gamma > 3$.

The conserved dynamics of a solid surface growing under the action of an external flux of particles is described by the continuum equation

$$\partial_t z(x,t) = -\partial_x j(x,t) + \delta F(x,t) \tag{1}$$

where $z(x,t)$ is the local height of the surface in a comoving frame (so that the average value $\bar{z}$ is set to 0) and $\delta F(x,t)$ is the shot noise.

Thermodynamic and kinetic mechanisms contribute to j and its actual expression depends on the details of the growth process. Here we are interested in the growth of a high-symmetry surface by molecular beam epitaxy, where the instability has a purely kinetic origin: the reduced interlayer diffusion [1]. Nonetheless, our treatment will be as general as possible.

A wide class of models is described by the current

$$j = Km''(x) + j_{\mathrm{ES}}(m) \tag{2}$$

where $m = \partial_x z$ is the local slope. The first term generally describes a thermally activated relaxation of the surface, but kinetic mechanisms can also contribute to K [2].

The second term is responsible for the instability and its origin is an asymmetry in the sticking process of an adatom to a step (the Ehrlich–Schwoebel (ES) effect): sticking from the upper terrace is hindered and this implies an uphill current [3] which is called the ES current (j_{ES}). Also, other (generally stabilizing) processes can contribute to j_{ES} and this explains the different expressions j_{ES} may take [4].

Whatever these processes are, j_{ES} is linear in m at small slopes ($j_{\mathrm{ES}} \sim \nu m$) and therefore in the early stages of the growth it prevails on the first term (Km'') at sufficiently large wavelengths.

* Dedicated to the Peanuts cartoon strip on the occasion of its 50th birthday.

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This means that the linear stability of the flat surface will be decided by the sign of ν, a positive one meaning instability. In fact, in the limit $m \to 0$ we have

$$\partial_t z = -K\partial_x^4 z - \nu\partial_x^2 z \tag{3}$$

whose solution is $z(x,t) = \exp(\omega_q t)\cos(qx)$ with $\omega_q = \nu q^2 - Kq^4$. An uphill current means that j_{ES} has the same sign as the slope, so ν is positive and the flat surface is unstable ($\omega_q > 0$) against modulations of wavevector smaller than $\bar{q} = \sqrt{\nu/K}$; the instability appears after a typical time of order $t^* \simeq (\nu\bar{q}^2)^{-1} = K/\nu^2$.

The later evolution of the surface depends on the nonlinear form of the unstable current $j_{\mathrm{ES}}(m)$. By taking the spatial derivative of (1), we obtain

$$\partial_t m = \partial_x^2(-j) + \partial_x(\delta F) \tag{4}$$

and a parallel with a phase-ordering process is easily made, once we remark that the current can be obtained by a pseudo free energy $\mathcal{F}$:

$$j = -\frac{\delta\mathcal{F}}{\delta m} \qquad \mathcal{F}[m] = \int \mathrm{d}x \left[\frac{K}{2}(\partial_x m)^2 + V(m)\right] \qquad V'(m) = -j_{\mathrm{ES}}(m). \tag{5}$$

The instability of the flat surface ($j'_{\mathrm{ES}}(0) > 0$) means that the potential $V(m)$ has a maximum in $m = 0$ ($V''(0) < 0$). Contiguous regions of increasing and opposite slope are formed. The usual phase-ordering process is obtained when $V(m)$ has the classical double-well form: $V(m) = -(\nu/2)m^2 + (\nu/4m_0^2)m^4$, corresponding to a current $j_{\mathrm{ES}} = \nu m(1 - m^2/m_0^2)$. After the slope has attained a fraction of m_0 the dynamics enters in the nonlinear regime: the wavelength L of the profile increases in time (coarsening process) and the slope saturates to the constant values $\pm m_0$. The coarsening law is known to be logarithmic [5] ($L(t) \sim \ln t$) in the absence of shot noise and a power law [6] ($L(t) \sim t^{1/3}$) in the presence of it.

The aim of this paper is to analyse the *deterministic* ($\delta F(x,t) \equiv 0$) growth process when $V(m)$ has no minima, corresponding to the absence of zeros at finite slopes in the current j_{ES}. We will consider the class of currents defined by

$$j_{\mathrm{ES}} = \frac{\nu m}{(1 + \ell^2 m^2)^\alpha} \qquad \text{with} \quad \alpha \geqslant 1 \tag{6}$$

and the corresponding models will be termed α models.

Model 1 has been studied numerically by Hunt *et al* [7] and they found a coarsening exponent $n \approx 0.22$ ($L(t) \sim t^n$) which seems not to depend on the noise strength (L M Sander, private communication). α models without noise have been studied analytically by Golubović [8] through scaling arguments and he finds $n = \frac{1}{4}$ irrespectively of α. Finally, qualitative considerations based on noise effects [9] give $n = 1/(2/\alpha + 3)$, i.e. $n = \frac{1}{5}$ for model 1.

Our analytical approach is based on the linear stability analysis of the stationary configurations $j[m(x)] \equiv 0$. In this way, one can find the coarsening exponent n through the determination of the lowest eigenvalue of the operator $(-\partial_x^2)\hat{H}$, where $\hat{H}$ is the Hamiltonian corresponding to a particle in a periodic potential [5].

Before proceeding, we render adimensional the growth equation by rescaling x with $1/\bar{q}$, t with t^* and z with $1/\bar{q}\ell$:

$$\partial_t z = -\partial_x j \qquad j = m'' + \frac{m}{(1 + m^2)^\alpha}. \tag{7}$$

Stationary configurations are the solutions of the differential equation $j[m(x)] = m'' + j_{\mathrm{ES}}(m) \equiv 0$. Therefore, they correspond to the periodic orbits of a particle in the potential $-V(m) = -[\frac{1}{2}(\alpha - 1)](1 + m^2)^{1-\alpha}$ for $\alpha > 1$ and in the potential $-V(m) = (\frac{1}{2})\ln(1 + m^2)$ for $\alpha = 1$. In the former case the potential is upper bounded and the solution corresponding

to the boundary conditions $m \to \pm\infty$ when $x \to \pm\infty$ does exist, while it does *not* for $\alpha = 1$ because the corresponding energy would be infinite. Stationary solutions may be labelled with their period, i.e. the wavelength L: $m_L(x)$.

Let us now perform a linear stability analysis around these stationary and periodic solutions: $m(x,t) = m_L(x) + \psi(x,t)$. It is easily found that

$$\partial_t \psi = \partial_x^2[-\psi''(x,t) + U_L(x)\psi] \tag{8}$$

where $U_L(x) \equiv -j'_{\mathrm{ES}}(m_L(x))$. By putting $\psi(x,t) = \phi(x)\exp(-\epsilon t)$ we obtain

$$(-\partial_x^2)[-\phi''(x) + U_L(x)\phi] \equiv D_x \hat{H}\phi(x) = \epsilon\phi. \tag{9}$$

Negative eigenvalues mean that $m_L(x)$ is linearly unstable and this induces the coarsening process; moreover, $\epsilon(L) \to 0^-$ when $L \to \infty$. The dependence of the ground state (GS) energy on the distance L determines the timescale of the coarsening process: $t \sim 1/|\epsilon(L)|$. For the moment we will assume $D_x \equiv 1$, i.e. we will consider the *nonconserved* model: $\partial_t m = -\delta\mathcal{F}/\delta m$.

First of all we observe that in the limit of large L the energy shift $\epsilon(L)$ for the periodic potential is equal (up to a numerical factor) to the shift for a single couple of potential wells†. The solution of the problem is given [11] in terms of ϕ_0 and ϕ_1, respectively the GS for the single well $U_1(x)$, centred in $x = L$, and for the double well $U_2(x)$, centred in $x = \pm L$. In fact, the Schrödinger equations are

$$-\phi_0'' + U_1\phi_0 = 0 \tag{10a}$$

$$-\phi_1'' + U_2\phi_1 = \epsilon\phi_1 \tag{10b}$$

and by evaluating the quantity $\int_0^\infty \mathrm{d}x\,[\phi_1 \times (10a) - \phi_0 \times (10b)] = 0$, we obtain

$$\phi_1(0)\phi_0'(0) = -\epsilon \int_0^\infty \mathrm{d}x\,\phi_0(x)\phi_1(x) \tag{11}$$

where we have made use of $U_1 = U_2$ for $x > 0$.

Before proceeding we must determine the asymptotic expressions of $\phi_0(x)$ and $\phi_1(x)$. The potential $U(x) = -j'_{\mathrm{ES}}(m)$ is given, for α models, by

$$U(x) = \frac{(2\alpha-1)m^2 - 1}{(1+m^2)^{\alpha+1}} \to \frac{(2\alpha-1)}{m^{2\alpha}}. \tag{12}$$

The asymptotic behaviour of the single-mound profile is obtained by integrating the equation $m''(x) + j_{\mathrm{ES}}(m) = 0$ and taking the limit $x \to \infty$:

$$(\tfrac{1}{2})(m')^2 - V(m) = 0 \Rightarrow \frac{\mathrm{d}m}{\mathrm{d}x} \approx \frac{1}{\sqrt{\alpha-1}}\frac{1}{|m|^{\alpha-1}}. \tag{13}$$

The result $m^\alpha(x) \approx (\alpha/\sqrt{\alpha-1})x$, when inserted in (12) gives

$$U(x) \approx \frac{(2\alpha-1)(\alpha-1)}{\alpha^2}\frac{1}{x^2} \equiv \frac{a}{x^2} \tag{14}$$

with a increasing between $a = 0$ (for $\alpha = 1$) and $a = 2$ (for $\alpha = \infty$).

The solution of the Schrödinger equation (10*a*) for $U_1(x) \approx a/(x-L)^2$ gives a *power-law* decaying wavefunction ($\phi_0(x) \sim |x-L|^{-\beta}$), with an exponent $\beta = (1 - 1/\alpha)$.

If $\alpha \leqslant 2$ then $\beta \leqslant \frac{1}{2}$ and therefore the GS $\phi_0(x)$ of the single well is not a bound state, since $\int_{-\infty}^{\infty} \mathrm{d}x\,\phi_0^2(x) = \infty$. On the other hand, for $\alpha > 2$ $\phi_0(x)$ is a bound state and $\phi_1(x)$ can

† If ϵ_2 is the energy shift for a couple of wells, the shift ϵ_n for n wells is $\epsilon_n = 2\epsilon_2(1 - 1/n)$.

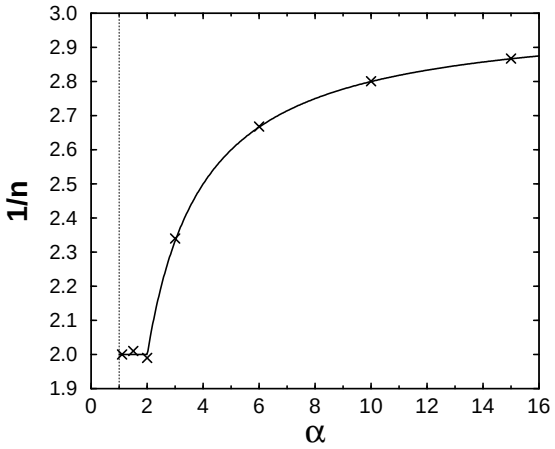

Figure 1. Analytical (full curve) and numerical (crosses) values for the exponent $1/n$ governing the asymptotic energy shift $|\epsilon_2| \sim 1/L^{1/n}$ (nonconserved model).

be approximated [11] with the expression $\phi_1(x) = [\phi_0(x)+\phi_0(-x)]/\sqrt{2}$. This way, from (11), we easily obtain the relation

$$\epsilon \simeq -2\phi_0(0)\phi_0'(0) \approx -L^{-(2\beta+1)} \qquad [\alpha > 2 \text{ and } D_x = 1]. \tag{15}$$

If $\alpha < 2$, we can put $\phi_1(x) = [\tilde{\phi}_0(x)+\tilde{\phi}_0(-x)]/\sqrt{2}$ where $\tilde{\phi}_0$ is a generalization of ϕ_0 to a negative eigenvalue: $-\tilde{\phi}_0''(x) + (a/x^2)\tilde{\phi}_0(x) = \epsilon\tilde{\phi}_0(x)$. In fact, even if ϕ_0 is not a bound state, ϕ_1 is bounded, because the GS energy ϵ is strictly lower than $U_2(\pm\infty) = 0$. The previous expression for ϕ_1 may be used even if ϕ_0 itself is bounded (i.e. for $\alpha > 2$) and the result for the coarsening exponent does not change.

The asymptotic expression for $\tilde{\phi}_0$ is $\tilde{\phi}_0(x) = \sqrt{x}K_\mu(\sqrt{|\epsilon|}x)$ where K_μ is the modified Bessel function of order $\mu = \beta - (\frac{1}{2})$. The function $\tilde{\phi}_0$ decays as a power law ($\tilde{\phi}_0(x) \approx |\epsilon|^{-\beta/2-1/4}x^{-\beta}$) if $a/x^2 \gg |\epsilon|$ and exponentially ($\tilde{\phi}_0(x) \approx |\epsilon|^{-1/4}\exp(-\sqrt{|\epsilon|}x)$) in the opposite limit, $a/x^2 \ll |\epsilon|$. Equation (11) now gives us

$$\epsilon \int_0^\infty \mathrm{d}x\, \phi_0(x)\tilde{\phi}_0(x) = -2\tilde{\phi}_0(0)\phi_0'(0) \qquad [\alpha \leqslant 2 \text{ and } D_x = 1] \tag{16}$$

where $\tilde{\phi}_0(x)$ depends on ϵ. Note that the integral I on the left-hand side does converge even if ϕ_0 is not a bound state.

The evaluation of the two sides of (16) is a bit lengthy and we report here the result only: $|\epsilon|\ln(1/|\epsilon|) \sim 1/L^2$ if $\alpha = 2$ and $|\epsilon| \sim 1/L^2$ if $1 < \alpha < 2$. In figure 1 we compare the analytical results for the exponent characterizing the energy shift $|\epsilon(L)| \sim L^{-1/n}$ with those obtained through its direct numerical evaluation† and the agreement is very good.

Therefore, for the nonconserved model we can conclude that

$$\text{(nonconserved)} \qquad n = \tfrac{1}{2} \quad (1 < \alpha \leqslant 2) \qquad \text{and} \qquad n = \frac{1}{3 - 2/\alpha} \quad (\alpha > 2) \tag{17}$$

with a logarithmic correction for $\alpha = 2$ ($L \sim (t/\ln t)^{1/2}$).

The reason why the coarsening exponent n keeps constant for $\alpha < 2$ is the following: if $\alpha > 2$ the single-well wavefunction is a bound state, the integral I is a constant while the 'superposition' between $\phi_0(x)$ and $\phi_0(-x)$ (that is to say the right-hand side of (16)) decreases at increasing α, which implies a decreasing n. Conversely, when $\alpha < 2$ the integral

† We have considered the single-well potential $U(x) = -E_0$ for $|x| < 1$ and $U(x) = a/x^2$ for $|x| > 1$, where $E_0(a)$ is chosen so as to provide a zero GS energy. Afterwards the energy ϵ_2 of the double well problem may be determined by joining the solutions of the Schrödinger equation in each separate 'piece' of the potential $U_2(x)$.

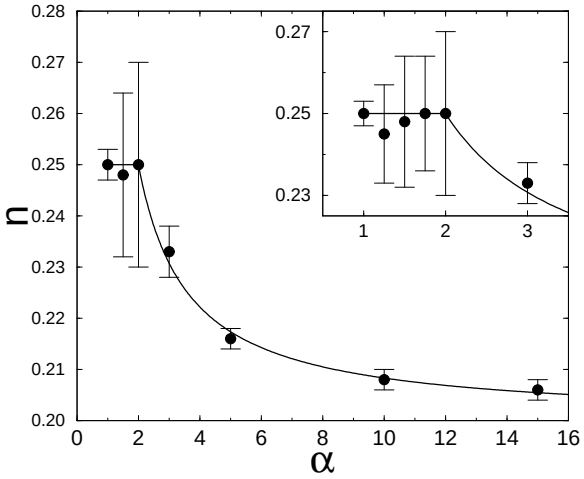

Figure 2. Coarsening exponent n for the conserved model. In the inset we enlarge the small-α region. The full curve is the analytical result (18). Points are the exponents found by integrating numerically (7) for a system size $M = 1024$ (spatial resolution $\Delta x = 0.25$) and a total time $400\,000 < T < 1600\,000$ (time step: $\Delta t = 0.05$). A few tests have also been done with a smaller time step ($\Delta t = 0.025$) and longer chains ($M = 2048$–4096), obtaining consistent results. Bars indicate the numerical fit errors.

I becomes α-dependent and decreases with α: this dependence counterbalances the reduction of the right-hand side of (16).

For the *conserved* growth model, $D_x = -\partial_x^2$ and (11) must be replaced by a more complicated expression. It has not been possible to carry out a rigorous calculation because $[\phi_1 \times D_x \hat{H}\phi_0 - \phi_0 \times D_x \hat{H}\phi_1]$ is no longer integrable. Nonetheless, there are strong indications that the right-hand sides of (15), (16) acquire a factor L^{-2}: the origin of this scaling factor is that $\phi_0(x)$ has a power-like behaviour (and therefore derivation corresponds to dividing by x) and also that $U(x) \sim x^{-2}$. Furthermore, since we need the single-well wavefunction, corresponding to a zero energy, a solution of the Schrödinger equation $\hat{H}\phi(x) = 0$ is also solution of $D_x \hat{H}\phi(x) = 0$.

As a consequence of such a factor, the coarsening exponent for the conserved case is easily obtained from the nonconserved one: $(1/n) \to [(1/n) + 2]$. Therefore,

$$\text{(conserved)} \qquad n = \tfrac{1}{4} \quad (1 < \alpha \leqslant 2) \qquad \text{and} \qquad n = \frac{1}{5 - 2/\alpha} \quad (\alpha > 2). \tag{18}$$

In order to check numerically the validity of the results reported in (18) and therefore the dependence of the coarsening exponent n on the parameter α, detailed numerical simulations have been performed. In particular, we have numerically integrated equation (7) by employing a pseudospectral time-splitting code†.

The values of $L(t)$, whose log–log plot gives the exponent n, are evaluated through the power spectrum (PS) of $z(x, t)$: the weighted average of the wavevectors corresponding to the most relevant components of the PS is $2\pi/L(t)$. A different method using the spatial correlation function gives consistent results. In figure 2, the numerical findings for $n(\alpha)$ by direct integration of (7) are shown together with the theoretical expression (18) and a good agreement is found.

In conclusion, we have found the analytic expression for the coarsening exponents $n(\alpha)$, both for the nonconserved model (17) and for the conserved one (growth model), (18). Coarsening varies with α and it is not logarithmic (i.e. $n = 0$) even for $\alpha = \infty$.

† The algorithm here employed is analogous to the leapfrog scheme introduced in [10] for the integration of the complex Ginzburg–Landau equation (CGLE). Here the integration of the nonlinear term cannot be treated analytically as for the CGLE, so we resort to a second-order Adams–Bashford scheme. A detailed discussion of these types of algorithms can be found in [12].

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