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Coarsening in an interfacial equation without slope selection revisited: Analytical results

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ABSTRACT

In this Letter, we re-examen a one-dimensional model of epitaxial growth that describes pyramidal structures characterized by the absence of a preferred slope [L. Golubović, Phys. Rev. Lett. 78 (1997) 90]. A similarity approach shows that the typical mound lateral size and the interfacial width growth with time like $t^{1/2}$ and $t^{1/4}$, respectively. This result was previously presented by Golubović. Our contribution provides a mathematical justification for the existence of similarity solutions which correspond to, or predict, the typical coarsening process.

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1. Introduction

In this Letter, we are concerned with the dynamics of a molecular beam epitaxy (MBE) growth model inducing pyramidal structures [1–7]. In this context, an analytical approach has been developed by Golubović [8]. In the Cartesian coordinates $x = (x, y)$, the standard phenomenological evolution equation for the continuous interfacial height h is of the form

$$\partial_t h + \nabla J = 0. \tag{1}$$

The expression of the surface current J is [5]

$$J(\nabla h) = a\frac{\nabla h}{1+|\nabla h|^2} + b\nabla(\Delta h), \tag{2}$$

where a and b are positive physical parameters. We assume, without any essential physical changes, that $a = b = 1$. The first term of J, the Ehrlich–Schwoebel (ES) barrier, is the destabilizing surface which has the form discussed by Johnson et al. [3]. The destabilizing term is balanced by the classical stabilizing linear term à la Mullins; $J_{stab}(\nabla h) = \nabla(\Delta h)$. This linear term describes relaxation through adatom diffusion driven by the surface free energy.

For the interface slopes $|\nabla h| \gg 1$ (i.e., terrace width $\ll$ distance between island nuclei), the destabilizing term reduces to the form suggested by Villain [1]; $J_{dest} = \frac{\nabla h}{|\nabla h|^2}$. This is the line advocated in [8], and consists to replace, for analytical study, Eqs. (1) and (2) by the equation

$$\partial_t h = -\nabla \frac{\nabla h}{|\nabla h|^2} - \Delta^2 h. \tag{3}$$

In the opposite limit, $|\nabla h| \ll 1$, Eqs. (1) and (2) can be linearized. Using the dispersion relation, we may see that there exists a band of unstable modes with wavelengths larger than $\lambda_c = 2\pi\sqrt{b/a} = 2\pi$, and with a fastest growing wavelength $\sqrt{2}\lambda_c$. Hence, perturbations with wavelengths smaller than λ_c are stabilized, whereas long-wavelength perturbations exponentially grow with time without bound, which lead to the strongly nonlinear regime (3).

For simplicity we limit ourselves here to $1+1$ dimensions. Eq. (3) reads

$$\partial_t h = -\partial_x\left(\frac{1}{\partial_x h} + \partial_x^3 h\right). \tag{4}$$

Such equation arises in various physical situations. For example it was derived by Paulin et al. [9] in the context of meandering instability. The destabilizing term is, of course, proportional to the step length, i.e., $J_{dest} = 1/\partial_x h$ (inverse Schwoebel effect). The same form has been found by Stoyanov [10] for electromigration of adatoms during growth without desorption. Without the relaxation term Eq. (4) was used in the continuum theory of mound formation in the case when interlayer is completely suppressed, and nucleation on the vicinal terrace can be neglected (see [11,12] and Section 3 below).

Despite the different physical context, an unified result is presented in [8] and [9] to describe the coarsening dynamics (see also [12] and the recent paper [13]). It is argued that the characteristic length scale of the surface $\lambda(t)$ and its typical height $H(t)$ grow with time as t^α and t^β, respectively, where

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$$\alpha = 1/4 \quad \text{and} \quad \beta = 1/2. \tag{5}$$

The singular equation (4) is a closely related more general equation

$$\frac{\partial h}{\partial t} = -a\frac{\partial}{\partial x}m^{\rho} - b\frac{\partial^3}{\partial x^3}m^n, \tag{6}$$

where $m = \partial_x h$ is the surface slope. This equation, with $a\rho > 0$ and $b > 0$, is proposed by Pimpinelli et al. [14] in the context of a classification schema for step bunching instabilities. The authors showed that the characteristic scaling exponents are $\alpha = \frac{n-\rho}{2(n+1-2\rho)}$ and $\beta = \frac{2+n-\rho}{2(n+1-2\rho)}$, which lead to (5) for $n = 1$ and $\rho = -1$ (see also [15]).

Since we regard these exponents as physically relevant, it is the purpose of the present Letter to re-examen some remarkable features of the singular interfacial model. Our aim here is not to introduce another intuitive or speculative physical scenario. Rather, an effort is made to report on an analytical justification of solutions to Eq. (4) which correspond to, or predict, the typical coarsening process. In fact, we are mainly concerned with similarity solutions to Eq. (4) and with its geometrical properties. In particular, we shall establish that there are solutions to (4) with $\partial_x h = 0$ at some points (x_0, t_0) where $\partial_{xx} h$ blows up. Moreover, $h(x,t)$ behaves as

$$h(x,t) \sim \left(\frac{t}{t_0}\right)^{1/2} h(x_0, t_0) \pm \frac{1}{2}\left(x - t^{1/4}\eta_c\right)^2 \sqrt{\left|\ln\left(xt^{-1/4} - \eta_c\right)^2\right|},$$

as $(x,t) \to (x_0, t_0)$, where $\eta_c = x_0 t_0^{-1/4}$.

2. Formulation of the problem

Since analytical solutions to (3) are difficult to extract, Golubović [8] examined the coarsening behavior by using a phase ordering type theory. The idea is to assume that the height function can be written in the form

$$\langle h(\mathrm{x}_0 + \mathrm{x}, t) h(\mathrm{x}_0, t)\rangle = H^2(t)\phi\left(\frac{\mathrm{x}}{\lambda(t)}\right), \tag{7}$$

where ϕ is some structure characterizing the phase ordering process and the angular brackets represent a spacial average. It is proved that the typical mound lateral size and the interface width behave as

$$\lambda(t) \sim t^{\alpha}, \qquad H(t) \sim t^{\beta},$$

for large t, where the coarsening and roughness exponents α, β are given by (5), irrespective of the interface dimension.

Using the similarity ansatz

$$h(x,t) = t^{\beta} f(\eta), \quad \eta = xt^{-\alpha}, \tag{8}$$

Paulin et al. [9] obtained that the lateral periodicity of the meander increases as $t^{1/4}$ (i.e., $h(x + \lambda(t), t) = h(x,t)$, where $\lambda(t) \sim t^{1/4}$).

The theoretical investigations of [8] and [9] do however not include the geometrical properties of the φ or f, which, from the mathematical view point, have to be added in the analysis for the coarsening process. In simple words, the scaling exponent α introduced in (8) is the coarsening exponent if the shape f is a periodic function. A second important question concerns the asymptotic behavior of the interfacial height h at a singular point (i.e., where $\partial_x h = 0$). These compose the main subject of the present work. This is the first time, where we are analytically faced with the oscillatory properties of the shape function for the coarsening dynamics. The analysis showed, as it is expected, that f is periodic and, in particular, indicated that there are solutions to Eq. (4) with singular points (i.e., $\frac{\partial h}{\partial x} = 0$), where their first derivatives are continuous. However, they do not have bounded second derivatives. The profile f is also used to study the asymptotic behavior of h in a neighborhood of any singular point.

Using the scaling assumption (8), where $\beta = 1/2$ and $\alpha = 1/4$, one sees that f needs to be a solution to the following non-autonomous singular ordinary differential equation (SODE for short)

$$f^{(iv)} - \frac{f''}{(f')^2} - \frac{1}{4}\eta f' + \frac{1}{2}f = 0, \quad \text{for } \eta \in \mathbb{R}, \tag{9}$$

where primes denote differentiation with respect to the similarity variable η. This is the equation we are going to deal with in Section 4.

It should be stressed that if we are appealing to seek a solution to Eqs. (1) and (2) having the similarity from (8) where $\beta > \alpha$ (no slope selection), we still have $\beta = 1/2$, $\alpha = 1/4$, but the new profile f satisfies (for the one-dimensional case)

$$f^{(iv)} + \left(\frac{f'}{t^{-1/2} + (f')^2}\right)' - \frac{1}{4}\eta f' + \frac{1}{2}f = 0. \tag{10}$$

It follows from this that the coarsening process of the original problem (1) and (2) cannot be inferred from the scaling argument. Nevertheless, in the limit of large t, i.e., when the term $t^{-1/2}$ becomes negligible compared to f'^2, Eq. (9) is an asymptotic form of Eq. (10). This may explain, as mentioned in [15], way it was necessary to go to extremely long times to find numerically the characteristic scaling exponents α and β from Eqs. (1) and (2) (see also [4] and [5]).

3. The Storm equation

In order to make the effect caused by the stabilizing term more transparent, we consider, in this short section, the singular interfacial equation in a limit where the relaxation term can be neglected; $J = J_{dest}$ [1,2,11]. In this event we revisit briefly the following equation

$$\partial_t h = \frac{\partial_{xx} h}{(\partial_x h)^2}, \tag{11}$$

or its spacial derivative

$$\partial_t m = \partial_x\left(m^{-2}\partial_x m\right), \tag{12}$$

which is often referred to as the Storm equation. There are several monographs which are devoted mainly to Eqs. (11) and (12).

Eq. (11) was proposed by Krug as a simple continuum (limit) model of a growing surface in which interlayer transport is completely inhibited [11]. It was also used to describe, for large t, the collective step meander on a vicinal surface [16]. Eq. (12) was found in 1951 by Storm [17], who showed, for the first time, that it could be reduced to the linear heat equation via a nonlocal transformation. Remarkably Eq. (11) has many exact solutions. Some of them are:

$$h_1(x,t) = \left[-2t\ln\left(4\pi tx^2\right)\right]^{1/2}, \tag{13}$$

provided $x(4\pi t)^{1/2} \in (0,1)$,

$$h_2(x,t) = \pm(t - \ln x), \tag{14}$$

for $x > 0$ and (separable solution)

$$h_3(x,t) = 2\sqrt{t}\,\mathrm{erf}^{-1}\left(1 - 4|x|/\lambda_s\right), \tag{15}$$

for $|x| < \lambda_s/2$, where the wavelength $\lambda_s > 0$ is arbitrary [12,11,16]. We may deduce from (15) that the interface width has the

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