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Different Regimes in the Ehrlich-Schwoebel Instability

Paolo Politi (*)

CEA-Grenoble, Département de Recherche Fondamentale sur la Matière Condensée,
SPMM/MP, 38054 Grenoble Cedex 9, France
Centre de Recherche sur les Très Basses Températures, CNRS, BP 166,
38042 Grenoble Cedex 9, France

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Abstract. — A one-dimensional high-symmetry growing surface in presence of step-edge barriers is studied numerically and analytically, through a discrete/continuous model which neglects thermal detachment from steps. The morphology of the film at different times and/or different sizes of the sample is analyzed in the overall range of possible step-edge barriers: for a small barrier, we have a strong up-down asymmetry of the interface, and a coarsening process — with an increasing size of mounds — takes place; at high barriers no coarsening exists, and for infinite barriers the up-down symmetry is asymptotically recovered. The transition between the two regimes occurs when the so-called Schwobel length is of order of the diffusion length.

1. Introduction

The stable growth mode of a high-symmetry surface in Molecular Beam Epitaxy is layer-by-layer growth: newly fallen adatoms diffuse on the surface till they meet a “trap”, which may be another adatom, or the step of a growing island. Afterwards, islands coalesce by leading to the completion of the layer, and the process starts again. Nevertheless, adatoms approaching a step from above may be hindered from descending it, because of step-edge barriers (Ehrlich-Schwobel effect [1]). This causes — on one side — a higher adatom density and therefore a higher probability of nucleation, and — on the other side — an up-hill current [2] (also called diffusion bias): both effects determine the formation of mounds.

If the main relaxation mechanism of the surface is surface diffusion and vacancies/overhangs can be neglected, the surface evolves by preserving the volume so that the following Langevin-type equation can be written for the local height $z(x, t)$:

$$\partial_t z = -\partial_x j + F + \eta. \quad (1.1)$$

(*) *Present address:* Dipartimento di Fisica, Università di Firenze, L.go E.Fermi 2, 50125 Firenze, Italy (e-mail: politip@fi.infn.it)

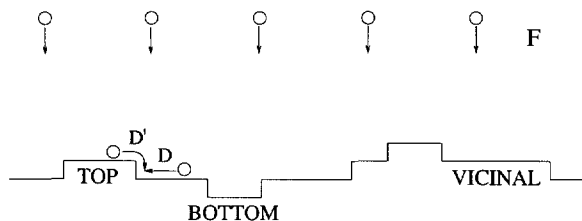


Fig. 1. — Profile of the one-dimensional high symmetry growing surface. F is the flux of particles (per unit time and unit surface). Top, vicinal and bottom terraces are indicated. D and D' are the sticking coefficients, from above (D') and below (D). Their asymmetry defines the Schwoebel length (see the text).

Here and throughout the paper, the lattice constant is put equal to one. F is the flux of atoms: it will be incorporated in z ($z \rightarrow z - Ft$). Finally, η is the noise, which may have different origins (shot noise, diffusion noise, nucleation noise). A most used expression for j is [3–5]:

$$j = j_s(m) + Km''(x) \quad m \equiv \partial_x z(x, t). \quad (1.2)$$

The first term will be called Schwoebel current and it is due to the above mentioned diffusion bias. It depends on the Schwoebel length, which is a measure of the asymmetry in the sticking coefficients to a step (see Fig. 1), from above (D') and below (D):

$$\ell_s = \left(\frac{D}{D'} - 1 \right). \quad (1.3)$$

Its actual form may have [4] or not [5, 6] zeros at finite slopes $m = \pm m^*$. In the former case, the growth equation (1.1) is equivalent to the Cahn-Hilliard equation, where m plays the role of order parameter:

$$\partial_t m = \partial_x^2 \left(\frac{\delta F}{\delta m} \right) + \partial_x \eta \quad (1.4)$$

$$F = \int dx \left[\frac{K}{2} (\partial_x m)^2 + U(m) \right] \quad U'(m) = -j_s(m). \quad (1.5)$$

So, the surface undergoes a spinodal decomposition process, with the formation of regions of size L , where the slope is alternatively in the two minima $m = \pm m^*$ of the potential $U(m)$. These regions are separated by domain walls and their typical size increases in time according to a power law: $L \sim t^n$. For a conserved order parameter, $n = 1/3$ [7] if η is due to shot-noise, while L increases logarithmically if η is absent [8]. In 2+1 dimensions, as pointed out by Siegert and Plischke [4], the growth equation has no exact counterpart in the Cahn-Hilliard equation (one reason is that \mathbf{m} satisfies the extra-condition: $\nabla \wedge \mathbf{m} = 0$), but the evolution is very similar and numerical solutions of the corresponding Langevin equation give [4] $n = 1/4$.

The previous scenario is expected to be valid if a strong term of the form $j = Km''(x)$ is present in the current, also at the largest slopes allowed by the dynamics. Such term was introduced by Mullins [9] to explain the relaxation of a grooved surface *via* surface diffusion. Its microscopic origin is thermal detachment from steps, and its form simply translates a current deriving from a chemical potential proportional to the surface curvature.

In the present article, we will study the opposite limit of a far from equilibrium system, when thermal detachment can be neglected (as found experimentally in Fe/Fe [10] at not too high temperatures), and other terms appear in the current.

A first important issue is the following: the current (1.2) changes sign if $z \rightarrow -z$, meaning that the resulting morphology is up-down symmetrical. This property is not always satisfied, neither in experiments [11, 12], nor in simulations [6, 13, 14]. So, a term of the form $j_c = \partial_x A(m^2)$, whose justification was given in reference [6], will be added: it has the simplest form which breaks the up-down symmetry, by keeping the reflection symmetry ($x \rightarrow -x$).

Even if thermal detachment is neglected, other mechanisms [6, 15] may contribute to a Mullins-like term in the current: for example, random nucleation and diffusion noise. In the limit of large terraces, random nucleation prevails [15], and only this one will be retained. However, since nucleations depend on the length of the terrace (see below), this means that K is indeed a function of the slope: $K = K(m)$, which vanishes if nucleation events are very rare. This is one of the main reasons why the resulting morphologies in a far from equilibrium system differ a lot from the quasi equilibrium case.

2. The Model

The discrete/continuous model which will be used throughout the paper was introduced by Elkinani and Villain [16]. In this model, a one-dimensional high-symmetry growing surface “contains” steps, but not adatoms, which are treated in a continuous way *via* a diffusion equation, whose boundary conditions at steps give step velocities.

The diffusion equation is integrated by an expression giving the probability of nucleation $P(\ell)$ per unit time on a given terrace of width ℓ . Let us briefly recall its form.

The probability $P(\ell)$ may be determined as the rate ($F\ell^d$) of incoming atoms on a terrace of dimension d ($d = 1, 2$) times the probability p for each adatom to meet another one (before sticking to a step). p is approximately given by the number of distinct sites visited by the adatom ($\sim \ell^d$, if logarithmic corrections are neglected) times the (average) density $\langle \rho \rangle$ of adatoms. Finally:

$$P(\ell) \approx F\ell^d \ell^d \langle \rho \rangle. \quad (2.1)$$

We want to stress that $\langle \rho \rangle$ depends on ℓ_s and on the type of terrace. By characterizing a terrace according to the number of ascending and descending steps (see Fig. 1), we will speak of top terraces (no ascending steps), vicinal terraces (both types of steps) and bottom terraces (no descending steps). Adatom density is not influenced by step-edge barriers on a bottom terrace, whilst on a top terrace $\langle \rho \rangle$ goes to infinity when $\ell_s \rightarrow \infty$, and this strongly increases the probability of nucleation $P(\ell)$ (see the Appendix).

For a weak Schwoebel effect we can neglect the dependence of $\langle \rho \rangle$ on ℓ_s and the solution of the diffusion equation gives $\langle \rho \rangle \approx F\ell^2/D$, so that

$$P(\ell) \approx \frac{F^2 \ell^{2(d+1)}}{D} \quad (2.2)$$

We define nucleation length the typical linear size of a terrace just before a nucleation process takes place, or — in other words — as the typical size of a terrace for which the probability of nucleation during the deposition of one layer ($t = 1/F$) is of order one: $P(\ell)/F \approx 1$. For a bottom terrace, or — equivalently — in the submonolayer regime, we will use alternatively the more common term of diffusion length (ℓ_d). So, from equation (2.2) we obtain

$$\ell_d \approx \left(\frac{D}{F} \right)^{\frac{1}{2(d+1)}} \quad (2.3)$$

This well-known result [17] is valid in the hypothesis that the nucleation of two adatoms is an irreversible process (not too high temperature) and that islands are not fractal (not too

low temperature). More details and the explicit expressions for the nucleation lengths of a top (ℓ_n^T), a bottom ($\ell_n^B \equiv \ell_d$) and a vicinal (ℓ_n^V) terrace are given in Appendix.

In this paper, the following general expression for the surface current will be used [18]:

$$j = j_s + j_c + j_K \equiv \frac{F\ell_s\ell_d m}{2(1 + \ell_s/\ell_d + |m|\ell_s)(1 + |m|\ell_d)} - \partial_x \left(\frac{F\ell_d^2}{8(1 + m^2\ell_d^2)} \right) + K(m)m''(x). \quad (2.4)$$

It is noteworthy that j_c does not depend on ℓ_s (see also Refs. [19,20]); on the other side, the actual dependence of K on ℓ_s and m is not exactly known. This equation will be exploited in the following sections to accompany the numerical simulations of the model described above.

3. Aim of the Paper

The aim of the present work is to study the different morphologies of a 1+1 dimensional growing surface which is strongly out of equilibrium. In this limit, it has been shown in reference [6] that deep crevasses appear at sufficiently long time/length scales.

The scenario given in reference [6] is representative of a low ℓ_s regime ($\ell_s \ll \ell_d$). In this case two critical wavelengths exist, a lower one (λ_c^{inf}) and an upper one (λ_c^{sup}). For scales smaller than λ_c^{inf} the flat surface is stable, but after a typical time t^* mounds develop with a size $L (= \lambda_c^{\text{inf}})$ which increases in time *via* a coarsening process. These mounds are not (up-down) symmetric and are separated by angular points.

When $L = \lambda_c^{\text{sup}}$ coarsening stops and deep crevasses form in between. It is noteworthy that the existence of the coarsening process may be explained in terms of the stability properties of stationary mounds, which exist in the interval $\lambda_c^{\text{inf}} < L < \lambda_c^{\text{sup}}$. mounds are stable with respect to height fluctuations (which means that they keep their form during coarsening) and unstable with respect to width fluctuations (which means that a large mound “eats” a smaller one).

When $L \rightarrow \lambda_c^{\text{inf}}$ the height of mounds goes to zero, meaning that the flat surface is stable at sufficiently small scales, while for $L \geq \lambda_c^{\text{sup}}$ mounds become unstable even for height fluctuations.

The case of infinite Schwoebel effect has been studied, for a far from equilibrium system, by Krug [19]. He asymptotically finds up-down symmetric configurations, which he calls “wedding cakes”. He also find their analytical profile, which is given by the inverse of the Error function.

In the following we will study the transition between the two regimes, by focusing on the following questions: i) is the scenario found in reference [19] for $\ell_s = \infty$ valid also for sufficiently large ℓ_s ? ii) how does the transition between the two regimes occur? iii) why at infinite ℓ_s is the up-down symmetry asymptotically recovered?

4. Results and Discussion

In the following we will call the behaviours described in reference [6] ($\ell_s \ll \ell_d$) and in reference [19] ($\ell_s = \infty$), respectively as “small- ℓ_s ” and “large- ℓ_s ” regimes. To understand how a transition between them can occur, let us focus on the upper critical wavelength. First of all, we will show that λ_c^{sup} is a decreasing function of ℓ_s .

If we adopt a purely deterministic point of view, according to which nucleation takes place on a terrace only when its width equals its nucleation length, we have a much simpler model

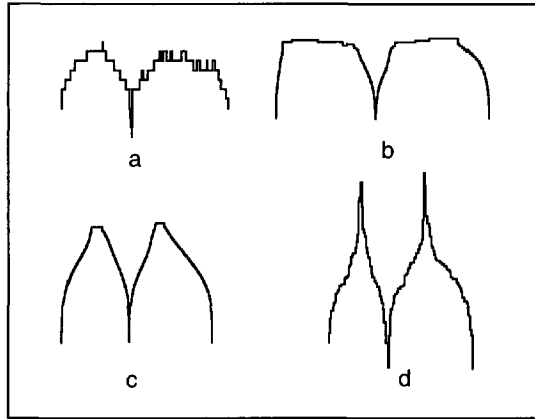


Fig. 2. — Typical morphologies of the surface at different values of the Schwoebel length ($\ell_s/\ell_d = 0.1$ (a), 1 (b), 100 (c), ∞ (d)). It is shown the transition from the small ℓ_s regime to the large ℓ_s one. Vertical and horizontal units are arbitrary. For the morphology (d), $t \simeq 400$ (in units of deposited layers), which results sufficiently long to recover the up-down symmetry. (The morphology at $\ell_s = \infty$ is drawn from Ref. [19], and the relative simulation data are a courtesy of Martin Schimschak.)

which is unable to explain λ_c^{inf} (whose origin is just random nucleation), but which can explain qualitatively well λ_c^{sup} . In the limit $|m| > 1/\ell_d$, the current (2.4) writes:

$$j = j_s + j_c \equiv \frac{F\ell_s m}{2(1 + |m|\ell_s)|m|} + \frac{F}{4m^3} \frac{\partial m}{\partial x} \quad (4.1)$$

The equation $j = 0$ can be solved if the “starting” slope m_0 is known. In a deterministic model m_0 is nothing but the inverse of the nucleation length of a top terrace (the only one where nucleation takes place). This way, we can write down the expression of λ_c^{sup} .

$$\lambda_c^{\text{sup}}|_{\text{det}} = \frac{[\ell_n^T(\ell_s)]^2}{8\ell_s} + \frac{\ell_n^T(\ell_s)}{2} \quad (4.2)$$

where we have stressed the ℓ_s dependence of ℓ_n^T . As detailed in Appendix, ℓ_n^T goes to zero when $\ell_s \rightarrow \infty$, so that λ_c^{sup} is a decreasing function of ℓ_s and $\lambda_c^{\text{sup}}(\infty) = 0$.

Anyway, the previous statement may be misleading, since the minimal meaningful length on a high symmetry surface is the diffusion length ℓ_d . In other words, the minimal distance between crevasses is set by the nucleations in the very first layers, which give rise to islands at an average distance ℓ_d (see, for example, Ref. [10]). Therefore λ_c^{sup} can not be smaller than this distance:

$$\lambda_c^{\text{sup}}(\ell_s) > \ell_d \quad \Rightarrow \quad \ell_s < \ell_s^{\text{sup}} \quad (4.3)$$

By using the deterministic formula (4.2) it is found $\ell_s^{\text{sup}} = 0.15\ell_d$ and $\ell_n^T(\ell_s^{\text{sup}}) = 0.8\ell_d$.

If $\ell_s > \ell_s^{\text{sup}}$ the flat surface is already unstable at the “minimal” scale ℓ_d . This morphology (see Fig. 2c) is rather similar to the one found by Krug [19] (see Fig. 2d) in the extreme case $\ell_s = \infty$, but while at finite ℓ_s an up-down asymmetry is maintained at all times, for $\ell_s = \infty$ the symmetry is asymptotically recovered. At this regard, a first trivial observation is that ℓ_n^T keeps finite for finite ℓ_s and it vanishes only for $\ell_s = \infty$. This implies that the top of the profile naturally differs from the bottom. On the other hand, the comprehension of the recovered up-down symmetry at large times for $\ell_s = \infty$ requires a more deep analysis.

Inspection of equation (4.1) shows that both j_s and j_c keep finite for $\ell_s = \infty$ (indeed, j_c does not depend on ℓ_s). Anyway, for $\ell_s > \ell_s^{\text{sup}}$ no stationary configuration exists and therefore there is no need for j_s and j_c to compensate.

Let us evaluate the ratio between the curvature term and the Schwoebel term, in the surface current (the slope m will be supposed to be positive):

$$\frac{j_c}{j_s} = \frac{m'}{2m^2} \left(\frac{1}{m\ell_s} + 1 \right). \quad (4.4)$$

For a strong Schwoebel effect, the ratio $(1/m\ell_s)$ is smaller than one and

$$\frac{j_c}{j_s} \simeq \frac{m'}{2m^2} = -\frac{\partial_x j_s}{F} = \frac{\partial_t z|_{j_c \equiv 0}}{F} \quad (4.5)$$

So, the condition $j_c \ll j_s$ is satisfied if the rate of growth ($\partial_t z$) of the surface, due to the Schwoebel current, is much smaller than the rate (F) of incoming atoms. (Let us remind that the “real” height of the surface is $z(x, t) + Ft$.)

We can check the previous condition by using the solution for $j_c \equiv 0$ [19]. The evolution equation $\partial_t z = Fz''/2(z')^2$ is separable and the differential equation can be solved: the profile is given by the inverse of the Error function and it is easily proved that

$$\frac{j_c}{j_s} \approx \frac{z}{2Ft} \quad (4.6)$$

Since the height $z(x, t)$ increases as \sqrt{t} , in the limit $t \rightarrow \infty$ the curvature term (j_c) is negligible with respect to the Schwoebel term (j_s). This means that the up-down symmetry is recovered, but only asymptotically.

After having discussed the region $\ell_s > \ell_s^{\text{sup}}$, let us turn to the region $\ell_s < \ell_s^{\text{sup}}$. In general terms, the lower critical wavelength λ_c^{inf} is determined by the linear stability analysis of the flat surface. In this case j_c ($\sim \partial_x m^2$ at small slopes m) is irrelevant and j has the form:

$$j = j'_s(0) m + Km''(x) \quad (4.7)$$

where $j'_s(0) = F\ell_s\ell_d/[2(1+\ell_s/\ell_d)]$. The exact expression of K is not known, but K surely does not increase with ℓ_s . For small (ℓ_s/ℓ_d) , dimensional analysis suggests the form $K = K_0 F \ell_d^4$, K_0 being a numerical constant [6].

The solution of the linear equation $\partial_t z = -\partial_x j$ gives the following expression for λ_c^{inf} .

$$\lambda_c^{\text{inf}} \sim 2\pi \sqrt{\frac{K}{j'_s(0)}} = 2\pi \sqrt{\frac{2K}{F\ell_d} \left(\frac{1}{\ell_d} + \frac{1}{\ell_s} \right)}. \quad (4.8)$$

So, λ_c^{inf} too is a decreasing function of ℓ_s . Furthermore, the limiting value does not depend too much on the actual form of K : if $K(\ell_s = \infty) = 0$, then $\lambda_c^{\text{inf}}(\ell_s = \infty) = 0$; conversely, if K has a weak dependence on ℓ_s ($K \approx K_0 F \ell_d^4$), then $\lambda_c^{\text{inf}}(\ell_s = \infty) = 2\pi \sqrt{2K_0 \ell_d}$. By comparison with the numerical results at small ℓ_s , where λ_c^{inf} is well defined (see Fig. 3), the determined value of K_0 gives rise to $\lambda_c^{\text{inf}}(\ell_s = \infty) \simeq 0.8/1.2 \ell_d$. Since lengths smaller than ℓ_d are meaningless, there is not a big difference between the two cases (constant K and decreasing K).

Now, what does happen to λ_c^{inf} , when ℓ_s is smaller, but of the same order of ℓ_s^{sup} ? Since by definition $\lambda_c^{\text{inf}} \leq \lambda_c^{\text{sup}}$, a second critical value ℓ_s^{inf} is expected, but two possibilities exist: $\lambda_c^{\text{inf}} = \lambda_c^{\text{sup}}$ (Fig. 3a) or $\lambda_c^{\text{inf}} = \ell_d$ (Fig. 3b), when $\ell_s = \ell_s^{\text{inf}}$ (The two possibilities coincide if $\ell_s^{\text{inf}} = \ell_s^{\text{sup}}$).

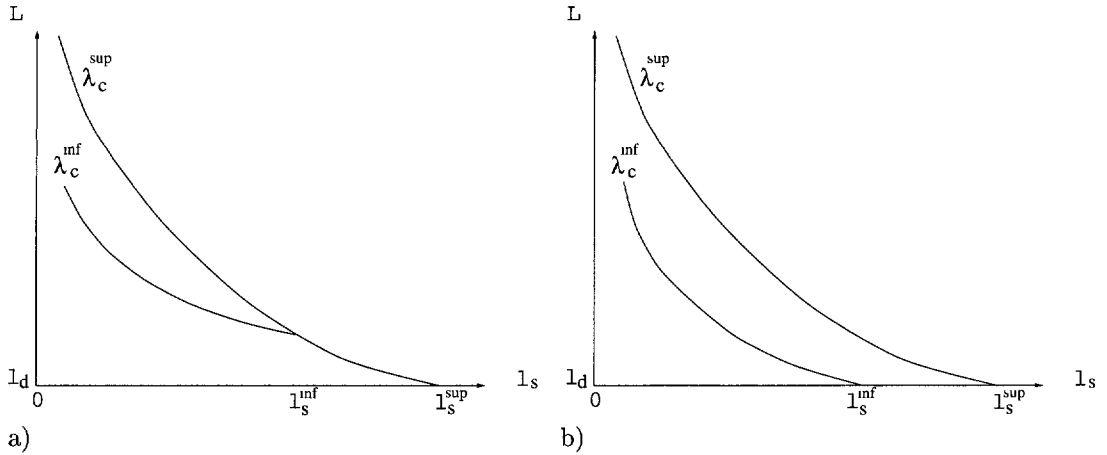


Fig. 3. — Schematic forms of the two possible “phase diagrams”. The coarsening region is in between the two curves. Note that ℓ_s varies in $[0, \infty]$, while L in $[\ell_d, \infty]$.

The evolution of the surface, in the interval $\ell_s^{\text{inf}} < \ell_s < \ell_s^{\text{sup}}$, differ in the two cases. In the former one, at increasing L (or the time t), we pass directly from a stable flat surface to an instability with formation of deep crevasses. In the latter case, mounds appear with a wavelength $\lambda = \ell_d$, we have coarsening, and afterwards the upper instability takes place. In other words, the flat surface is never stable (on scales larger than ℓ_d).

Which scenario really occurs is not evident. In fact, for $\ell_s \approx \ell_s^{\text{inf}}$ the coarsening region — if exists! — is very narrow and mounds have a typical size which is only slightly larger than ℓ_d . This means that fluctuations are very important, because nucleation events take place exactly on a length scale ℓ_d . A second difficulty is that λ_c^{inf} and λ_c^{sup} can not be located with extreme precision. λ_c^{sup} can be determined — for example — by changing the value of L (small size of the sample) and by checking when a mound is no more stable. Nevertheless, if $L \approx \ell_d$ stochasticity in nucleation makes the interface thickness $\Delta z (= z_{\text{max}} - z_{\text{min}})$ neither constant in time (meaning a stationary mound) nor constantly increasing in time (meaning an instability): rather, Δz shows an intermittent behaviour, with formation and healing of deep crevasses.

The location of λ_c^{inf} is even more difficult: some reasons were explained in reference [6], but here we will add a more pertinent comment. A continuum local equation results from a spatial average on a distance of order ℓ_d , so the notion of lower critical wavelength — which results from a linear stability analysis of the current (4.7) — breaks down if $\lambda_c^{\text{inf}} \simeq \ell_d$.

This happens just when $\ell_s \simeq \ell_s^{\text{inf}}$, therefore the difficulties in drawing the phase diagram (see Fig. 4) in the region $\ell_s \approx \ell_s^{\text{inf}}$, $L \approx \ell_d$.

In Figure 2, different morphologies, for different values of ℓ_s are shown: for $\ell_s/\ell_d = 0.1$ (Fig. 2a) we have mounds which would be stationary in absence of coarsening, and whose curvature is always negative. All the other structures (Figs. 2b, c, d) are unstable configurations, which are also characterized by the appearing of pieces of curve with a positive curvature. The size of the flat region, on the top, equals ℓ_n^T , which decreases at increasing ℓ_s . For $\ell_s = \infty$ this size vanishes, but the up-down symmetry appears only at large times.

In Figure 4, it is shown the “phase diagram” of the one-dimensional surface, in the plane $(\ell_s/\ell_d, L/\ell_d)$. The variable L may have two different meanings: for a small sample size, L is the sample size; for a very large sample, L is the typical size of the emerging structure. Because of the dynamics, this size increases in time, so L may even be thought as the “time”.

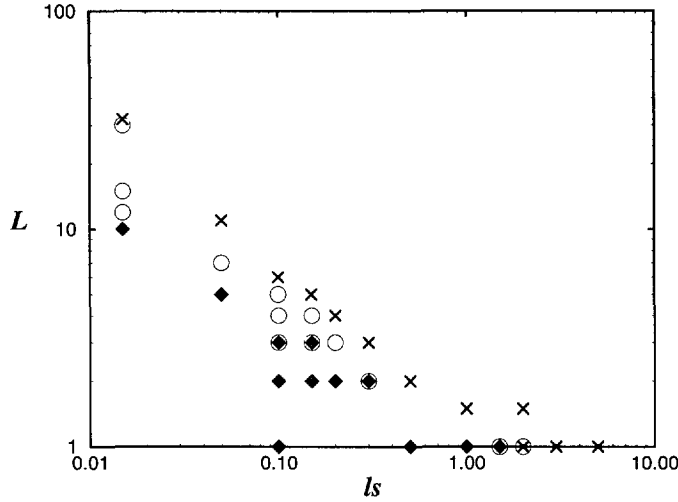


Fig. 4. — “Phase diagram” of the one-dimensional surface. Both ℓ_s and L are given in units of the diffusion length ℓ_d . The full rhombuses mean that the flat surface is stable; the circles that stationary mounds are present; the crosses that no stationary configuration exists and deep crevasses form. Other details are given in the text. For a given value of ℓ_s , if a cross is marked for $L = L_x$ then other crosses are present for all the $L > L_x$. Analogously, if a rhombus is marked for $L = L_\diamond$ then other rhombuses are present for $L < L_\diamond$.

The lower critical wavelength is located between full rhombuses and circles, and the upper one between circles and crosses. When two different symbols are superimposed, it means that it has not been possible to discriminate between them: for example, that it has not been possible to decide if the flat surface is stable or not, at the corresponding lengthscale. This occurs when $\ell_s \simeq \ell_s^{\text{inf}}$. From the figure, it is possible to locate ℓ_s^{sup} in the range $2/4 \ell_d$.

5. Conclusions

We have studied a one-dimensional high-symmetry surface, whose growth — in presence of step-edge barriers — is unstable (Ehrlich-Schwoebel instability).

If the flux is not too high and thermal detachment from steps is effective, current (1.2) should be relevant and the picture given in previous works [3, 4] applies. In this case, the up-down asymmetry is weak and the actual value of the Schwoebel length should not influence qualitatively the resulting morphology; nonetheless, it determines how long the crystal surface keeps flat.

In this paper we have studied the opposite limit of a far from equilibrium surface. Even if thermal detachment is absent, a Mullins-like term in the surface current is induced by random nucleation, so the *linear* description of the surface evolution is the same as in the quasi-equilibrium case.

When slope increases, a strong up-down asymmetry in the surface profile appears: it is a consequence of the nonlinear symmetry breaking term, but also of the inability of random nucleation to heal the surface at large slopes. Furthermore, the morphology of the growing crystal — at variance with the quasi-equilibrium case — depends on the value of the Schwoebel length, and for $\ell_s = \infty$, the up-down symmetry is asymptotically recovered.

The main features of the present model are i) the neglect of thermal detachment, and ii) the vanishing of the lattice constant a (continuum limit). The former determines an upper critical wavelength, the latter that slope can go to infinity. In reference [6] we have argued that λ_c^{sup} should survive even if i) is relaxed, if detachment is weak. Anyway, it will be important to study more carefully this point, so as to investigate the transition between the quasi-equilibrium case and the far from equilibrium one, treated here. We want also to stress that the existence of λ_c^{sup} does *not* depend on ii): in fact, the maximal slope at the angular points, just before the formation of deep crevasses, is weaker than $1/a$. Crystalline effects come into play after crevasses have appeared, and $m \simeq 1/a$.

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Appendix

Nucleation Lengths

The nucleation length ℓ_n of a terrace is determined by the condition (see Eq. (2.1)):

$$P(\ell_n) \cdot \frac{1}{F} = \ell_n^{2d} \langle \rho \rangle \approx 1 \quad (\text{A.1})$$

where $\langle \rho \rangle$ depends on the type of terrace.

The diffusion equation $F + D\rho''(x) = 0$ is solved in the interval $x \in (-\ell/2, \ell/2)$, with the following boundary conditions ($x = \pm\ell/2$):

$$\begin{aligned} \rho'(x) &= -\frac{1}{\ell_s} \rho(x) && \text{descending step} \\ \rho(x) &= 0 && \text{ascending step.} \end{aligned}$$

So, if $\ell_s = 0$ we need $\rho(x)|_{\text{step}} = 0$, because adatoms are automatically incorporated. For $\ell_s = \infty$, we have $\rho'(x)|_{\text{step}} = 0$.

It is found that (capital letters B, T, V refer — respectively — to a Bottom, a Top and a Vicinal terrace):

$$\begin{aligned} \rho_B(x) &= \frac{F}{2D} \left[\left(\frac{\ell}{2} \right)^2 - x^2 \right] \\ \rho_T(x) &= \frac{F\ell_s\ell}{2D} + \rho_B(x) \\ \rho_V(x) &= \frac{F\ell_s\ell}{2D(\ell_s + \ell)} \left(\frac{\ell}{2} - x \right) + \rho_B(x). \end{aligned}$$

It is manifest that $\rho_T \rightarrow \infty$ if $\ell_s \rightarrow \infty$, whilst ρ_V keeps finite. Finally, from (A.1) we obtain the following expressions/equations for the nucleation lengths, in 1+1 dimensions:

$$\ell_n^B \equiv \ell_d = \left(\frac{12D}{F} \right)^{1/4}$$

$$(\ell_n^T)^4 + 6\ell_s(\ell_n^T)^3 - \ell_d^4 = 0$$

$$(\ell_n^V)^5 + 4\ell_s(\ell_n^V)^4 - \ell_d^4(\ell_n^V + \ell_s) = 0.$$

For $\ell_s \gg \ell_d$, $\ell_n^T \simeq \ell_d(\ell_d/6\ell_s)^{1/3}$ and $\ell_n^V \simeq \ell_d/\sqrt{2}$.

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