Scalling properties of step bunches induced by sublimation, growth and electromigration : a unified perspective.

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Scaling properties of step bunches induced by sublimation and related mechanisms

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This work provides a ground for a quantitative interpretation of experiments on step bunching during sublimation of crystals with a pronounced Ehrlich-Schwoebel (ES) barrier in the regime of weak desorption. A strong step bunching instability takes place when the kinetic length $d_+=D_s/K_+$ is larger than the average distance l between the steps on the vicinal surface; here D_s is the surface diffusion coefficient and K_+ is the step kinetic coefficient. In the opposite limit $d_+ \ll l$ the instability is weak and step bunching can occur only when the magnitude of step-step repulsion is small. The central result are power law relations of the form $L \sim H^\alpha$, $l_{\min} \sim H^{-\gamma}$ between the width L, the height H, and the minimum interstep distance $l_{\min}$ of a bunch. These relations are obtained from a continuum evolution equation for the surface profile, which is derived from the discrete step dynamical equations for the case $d_+ \gg l$. The analysis of the continuum equation reveals the existence of two types of stationary bunch profiles with different scaling properties. Through comparison with numerical simulations of the discrete step equations, we establish the value $\gamma=2/(n+1)$ for the scaling exponent of $l_{\min}$ in terms of the exponent n of the repulsive step-step interaction, and provide an exact expression for the prefactor in terms of the energetic and kinetic parameters of the system. For the bunch width L we observe significant deviations from the expected scaling with exponent $\gamma=1-1/\alpha$, which are attributed to the pronounced asymmetry between the leading and the trailing edges of the bunch, and the fact that bunches move. Through a mathematical equivalence on the level of the discrete step equations as well as on the continuum level, our results carry over to the problems of step bunching induced by growth with a strong inverse ES effect, and by electromigration in the attachment/detachment limited regime. Thus our work provides support for the existence of universality classes of step bunching instabilities [A. Pimpinelli *et al.*, Phys. Rev. Lett. **88**, 206103 (2002)], but some aspects of the universality scenario need to be revised.

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I. INTRODUCTION

The formation of step bunches at a vicinal surface is a problem of great current interest, both from a fundamental viewpoint and with regard to the possible uses of step bunches as nanotemplates or nanostructures.[1–6] Mechanisms causing step bunching instabilities include strain effects,[1,2,7,8] sublimation under conditions of asymmetric detachment kinetics known as the Ehrlich-Schwoebel (ES) effect,[9–11] growth with an inverse ES effect,[9,12–14] and surface electromigration.[15–28]

Quite recently it was realized that step bunching is a promising way to study the interactions between the steps.[29–34] The physical ground is simple: The steps in the bunch keep a certain distance from each other because the step-step repulsion balances the tendency to further compression of the bunch. The free energy related to the step-step interaction is of the form A/l^n, where l is the interstep distance. When $n=2$, the amplitude $A(T)$ accounts for both elastic and entropic repulsion between the steps.[35] Under crystal-vapor equilibrium one has the relation $A(T) \sim g(T)$ where $g(T)$ is the step repulsion coefficient in the expression

$$f(\rho) = f(0) + \kappa\rho + g\rho^3 \tag{1}$$

for the surface free energy (per unit projected area) of a vicinal crystal surface with a density of steps ρ.

To infer information about the step-step interactions from experimental observations of bunch morphology, one makes use of scaling relations between the length and time scales characterizing the bunches. The relevant length scales are the width L and the height H of the bunch, and the spacing ξ between subsequent bunches (Fig. 1). The length ξ is also sometimes referred to as the terrace width; this nomenclature is somewhat ambiguous, however, because the region between two bunches may contain several monoatomic steps, and, hence, several wide terraces. The bunch height is related to the number of steps N in the bunch by $H=Nh_0$, where h_0 is the height of an atomic step. A quantity that is directly accessible to experimental observations[31] is the minimal terrace size $l_{\min}$ inside the bunch, which is related to the maximal slope $m_{\max}$ through $l_{\min}=h_0/m_{\max}$. Following the notation of Ref. 36, we introduce scaling exponents α and γ characterizing the shape of individual bunches through the relations

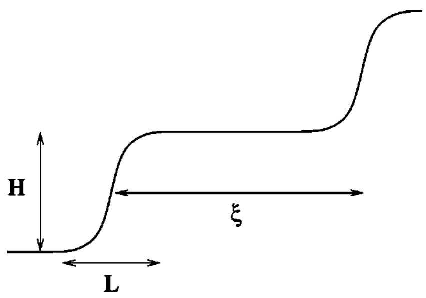

FIG. 1. Schematic of a bunched vicinal surface, illustrating the definition of the bunch width L, the bunch height H, and the bunch spacing ξ.

$$H \sim L^{\alpha}, \quad l_{\min} \sim N^{-\gamma}. \tag{2}$$

Assuming that the minimal terrace size $l_{\min}$ is of the same order as the mean size $\bar{l}=L/N$ of the terraces inside the bunch, one expects the exponent identity

$$\gamma = 1 - 1/\alpha. \tag{3}$$

Furthermore the coarsening of the bunch morphology with time is described by a dynamic exponent z defined through[36]

$$\xi \sim N \sim t^{\alpha/z}. \tag{4}$$

Because the ratio ξ/N must be equal to the mean terrace width l, which is fixed by the overall vicinality of the surface, the bunch spacing ξ and the bunch size N grow with time in the same manner.

For step bunching induced by surface electromigration, scaling relations of the form (2) have been derived both for nontransparent and transparent steps.[26,29,30,34] Their application to the analysis of experiments[31,32] proceeds in two stages. First, the value of the scaling exponent α or γ is used to determine the kinetic regime and the value of the step interaction exponent n, and subsequently an estimate for the strength of the step-step interaction (in relation to the driving force for step bunching) is extracted from the prefactor of the scaling relation. For example, for nontransparent steps one finds that $\alpha=(n+1)/(n-1)$, which yields $\alpha=3$ in the standard case $n=2$, whereas for $n=1$ the width of the bunch L would in fact be independent of the bunch size. Provided that $n=2$ and $\alpha=3$, the bunch width depends on the step interaction coefficient as $L\sim[A(T)]^{1/3}$. This relation provides a ground to study the temperature dependence of $A(T)$ by measuring the width of the bunch as a function of temperature.[33]

The main purpose of this paper is to derive scaling relations of the form (2) for step bunches induced by the ES effect during sublimation, and to put the results into perspective with regard to previous work on other step bunching instabilities. In the next section we introduce the basic concepts and quantities of the Burton, Cabrera, and Frank (BCF) model[37] in the presence of ES barriers (see Ref. 38 for a recent review). In Sec. III the equations of step motion are displayed and various limiting cases are discussed. In Secs. IV and V a continuum evolution equation for the surface is derived, and the structure of stationary bunch solutions is analyzed. A key result is the existence of two types of solutions with different scaling properties in the sense of (2). In Sec. VI the mathematical equivalence of the sublimation problem to appropriate limiting cases of step bunching induced by electromigration and growth with inverse ES barriers is pointed out and exploited. Section VII presents results obtained from numerical simulations of the discrete step dynamics and compares them to the predictions of the continuum theory. In Sec. VIII we critically examine[39] a recently proposed classification scheme for step bunching instabilities[36] in the light of our results, and some general conclusions are drawn in Sec. IX.

II. DISCRETE MODEL AND BASIC CONCEPTS OF SUBLIMATION BY STEP FLOW

We consider a vicinal surface going uphill in the $+x$ direction. The processes of atom migration (in the presence of desorption and deposition) are described by the stationary diffusion equation

$$D_s \frac{d^2 n_s}{dx^2} - \frac{n_s}{\tau_s} + R = 0, \tag{5}$$

where D_s is the coefficient of surface diffusion, n_s is the concentration of mobile atoms, adsorbed on the surface, R is the deposition rate of atoms to the crystal surface, τ_s is the lifetime of an atom in a state of mobile adsorption, and x is a coordinate perpendicular to the step edges (we consider a system of parallel steps with straight edges). The exchange of atoms between the crystal phase and the dilute layer of adatoms takes place at the steps and determines the boundary conditions for Eq. (5). It is essential to note that the ES barrier considerably decreases the permeability of the steps. Really, an atom must break many chemical bonds when it crosses over the step down to a position of adsorption at the step edge. Therefore, such an event happens very rarely. The opposite jump from the position of adsorption at the step edge to a position of adsorption on the upper terrace (or, briefly, from the lower to the upper terrace) also happens rarely in accordance to the principle of detailed balance. This circumstance justifies the reduction of the diffusion problem on the crystal surface to a diffusion problem at a single terrace. The boundary conditions relate the surface fluxes of adatoms with the power of the step as a generator (or a sink) of adatoms. For the terrace between the ith and $i+1$th step one can write

$$-D_s \left.\frac{dn_s}{dx}\right|_{x=x_i} = -K_-[n_s(x_i) - n_s^e(x_i)],$$

$$-D_s \left.\frac{dn_s}{dx}\right|_{x=x_{i+1}} = K_+[n_s(x_{i+1}) - n_s^e(x_{i+1})], \tag{6}$$

where K_+ and K_- are the kinetic coefficients for the ascending (K_+) and the descending (K_-) steps, respectively.[38] The step kinetic coefficients are defined by the expression for the velocity of the step motion

$$v=\frac{dx_i}{dt}=-a_\perp a_\parallel\{K_+[n_{s,i-1}(x_i)-n_s^e(x_i)]+K_-[n_{s,i}(x_i)-n_s^e(x_i)]\}, \tag{7}$$

where $a_\perp$ and $a_\parallel$ are the interatomic distances perpendicular and parallel to the steps, $n_{s,i-1}(x)$ is the adatom concentration on the terrace between the $i-1$th and the ith step, and $n_s^e(x_i)$ is the equilibrium value of the adatom concentration in the vicinity of the step, situated at x_i. The value of n_s^e in the vicinity of the ith step depends on the distances to the neighboring steps $i+1$ and $i-1$, since $n_s^e(x_i)=n_s^e\exp[\Delta\mu(x_i)/k_BT]$, where[29,30]

$$\frac{\Delta\mu(x_i)}{k_BT}=-\left(\frac{l_0}{x_{i+1}-x_i}\right)^3+\left(\frac{l_0}{x_i-x_{i-1}}\right)^3 \tag{8}$$

and

$$l_0=\left(\frac{2\Omega A(T)}{k_BT}\right)^{1/3} \tag{9}$$

is a length scale characterizing the strength of the step-step interaction. In (9) we have introduced the atomic area $\Omega=a_\perp a_\parallel$.

The Ehrlich-Schwoebel barrier[40] provides the physical ground for the inequality $K_-\neq K_+$, since the exchange of atoms between the crystal phase and the adlayer on the upper terrace has a lower rate than the exchange between the crystal and the adlayer at the lower terrace, i.e., $K_+>K_-$, although the opposite inequality has also been discussed.[41] Assuming that the step kinetic coefficients can be written in the form $K_\pm=K_0\exp(-E_\pm/k_BT)$ one can write $K_-/K_+=\exp(-\Delta E/k_BT)$ where $\Delta E=E_--E_+$ characterizes the asymmetry in the atom attachment-detachment kinetics at the steps. The ratio $\beta=K_-/K_+$ is an essential parameter in the considerations presented below.

III. EQUATIONS OF STEP MOTION

Since the normal ES barrier ($\Delta E=E_--E_+>0$) causes a step bunching instability only in the case of sublimation,[9] the equations of step motion will be derived under the condition $R=0$ (i.e., in the absence of deposition). The steps then move to the right. Solving the diffusion problem [Eq. (5) with the boundary conditions (6)] one obtains an expression for the adatom concentration at the crystal surface. Substituting $n_{s,i-1}(x_i)$ and $n_{s,i}(x_i)$ into Eq. (7) one can write an expression for the velocity dx_i/dt of the ith step as a function of the widths of the lower (left) and upper (right) terraces,

$$\frac{dx_i}{dt}=v_-+v_+. \tag{10}$$

In the physically interesting limit of small desorption rate, in the sense that the diffusion length $\lambda_s=\sqrt{D_s\tau_s}\gg x_{i+1}-x_i$, the two contributions to the step velocity (10) read

$$v_-=\frac{D_s\Omega n_s^e}{\lambda_s}\frac{\beta\left[\dfrac{\Delta\mu(x_i)}{k_BT}-\dfrac{\Delta\mu(x_{i+1})}{k_BT}\right]+\dfrac{\beta d_+}{\lambda_s}\left(\dfrac{x_{i+1}-x_i}{\lambda_s}\right)+\beta\left(\dfrac{x_{i+1}-x_i}{\lambda_s}\right)^2}{\dfrac{d_+}{\lambda_s}(1+\beta)+\left[\beta+\left(\dfrac{d_+}{\lambda_s}\right)^2\right]\left(\dfrac{x_{i+1}-x_i}{\lambda_s}\right)} \tag{11}$$

and

$$v_+=\frac{D_s\Omega n_s^e}{\lambda_s}\frac{\beta\left[\dfrac{\Delta\mu(x_i)}{k_BT}-\dfrac{\Delta\mu(x_{i-1})}{k_BT}\right]+\dfrac{d_+}{\lambda_s}\left(\dfrac{x_i-x_{i-1}}{\lambda_s}\right)+\beta\left(\dfrac{x_i-x_{i-1}}{\lambda_s}\right)^2}{\dfrac{d_+}{\lambda_s}(1+\beta)+\left[\beta+\left(\dfrac{d_+}{\lambda_s}\right)^2\right]\left(\dfrac{x_i-x_{i-1}}{\lambda_s}\right)}. \tag{12}$$

Here we have introduced the kinetic lengths[10,38] $d_+=D_s/K_+$ and $d_-=D_s/K_-=D_s/K_+\beta=d_+/\beta$. The equations (11) and (12) have two limiting cases,

$$\text{(a)}\quad \frac{d_+}{\lambda_s}(1+\beta)\ll\left[\beta+\left(\frac{d_+}{\lambda_s}\right)^2\right]\left(\frac{x_i-x_{i-1}}{\lambda_s}\right), \tag{13}$$

$$\text{(b)}\quad \frac{d_+}{\lambda_s}(1+\beta)\gg\left[\beta+\left(\frac{d_+}{\lambda_s}\right)^2\right]\left(\frac{x_i-x_{i-1}}{\lambda_s}\right). \tag{14}$$

The limit (a) (realized when $x_i-x_{i-1}\gg d_+$ and $d_+/\lambda_s\ll 1$) reduces the denominators of Eqs. (11) and (12) to $(\beta/\lambda_s)(x_i-x_{i-1})$. If in addition $\beta\gg(d_+/\lambda_s)^2$, the parameter β is eliminated from the terrace-length dependent destabilizing terms in (11) and (12), and appears only in a constant contribution to the step velocity, where it does not provide any ground for a step bunching instability. It is, however, quite possible that an instability is induced by higher order terms $[(x_i-x_{i-1})/\lambda_s]^\nu$ with $\nu>2$. We shall address this possibility in Sec. VII, devoted to numerical analysis of the discrete model.

The limit (b) is more interesting. It takes place under the assumption $x_i-x_{i-1}\ll d_+$ and $d_+/\lambda_s<1$. Then only the constant terms in the denominator of Eqs. (11) and (12) are retained and the terms quadratic in the terrace lengths can be neglected relative to the linear ones. Thus Eqs. (11) and (12) reduce to

$$v_- = \frac{D_s \Omega n_s^e}{d_+(1+\beta)}\left\{\frac{\beta}{k_B T}[\Delta\mu(x_i) - \Delta\mu(x_{i+1})] + \frac{\beta d_+}{\lambda_s^2}(x_{i+1} - x_i)\right\}, \quad (15)$$

$$v_+ = \frac{D_s \Omega n_s^e}{d_+(1+\beta)}\left\{\frac{\beta}{k_B T}[\Delta\mu(x_i) - \Delta\mu(x_{i-1})] + \frac{d_+}{\lambda_s^2}(x_i - x_{i-1})\right\}. \quad (16)$$

The two terms in the curly brackets have a clear physical meaning. The first term (the difference between the chemical potentials of neighboring steps) is the driving force for the relaxation of the fluctuations in the step density. The second term in Eqs. (15) and (16) reflects the asymmetry in the step kinetics and provides a ground for step bunching instability. These two terms describe a model previously analyzed in Ref. 42, where it was shown how continuum equations for the one-dimensional crystal profile $h(x,t)$ can be derived exactly, provided the step dynamics is linear in the terrace lengths. Indeed, neglecting the chemical potential difference in the square brackets, we can write

$$\frac{dx_i}{dt} = v_- + v_+ = \frac{D_s \Omega n_s^e}{\lambda_s^2}\left[\frac{\beta}{1+\beta}(x_{i+1} - x_i) + \frac{1}{1+\beta}(x_i - x_{i-1})\right], \quad (17)$$

where

$$\frac{D_s \Omega n_s^e}{\lambda_s^2} = \frac{\Omega n_s^e}{\tau_s} = \Omega R_e \equiv \hat{R}_e \quad (18)$$

is the equilibrium value of the desorption rate per adsorption site. We will return to the continuum equation derived from (17) below in Sec. V.

IV. CONTINUUM LIMIT OF THE RELAXATIONAL DYNAMICS

In this section we develop a continuum description for the relaxational part of the step dynamics. The chemical potential differences in Eqs. (15) and (16) can be written approximately in the form

$$\frac{1}{k_B T}[\Delta\mu(x_i) - \Delta\mu(x_{i-1})] \approx \frac{1}{k_B T}\left[\frac{\partial}{\partial x}(\Delta\mu)\right](x_i - x_{i-1}). \quad (19)$$

Making use of the relation $(x_i - x_{i-1}) \approx h_0(\partial h/\partial x)^{-1}$, one can bring the last expression into the form

$$\frac{h_0}{k_B T}\left(\frac{\partial h}{\partial x}\right)^{-1}\left[\frac{\partial}{\partial x}(\Delta\mu(x_{i-1}))\right]. \quad (20)$$

This is the contribution to the rate of motion of the ith step, due to the difference between the chemical potentials of the ith and the $i-1$th step. In the same way the contribution of the difference between the chemical potentials of the ith and $i+1$th step to the motion of the ith step is

$$-\frac{h_0}{k_B T}\left(\frac{\partial h}{\partial x}\right)^{-1}\left[\frac{\partial}{\partial x}(\Delta\mu(x_i))\right]. \quad (21)$$

Thus the total contribution of the variation of the chemical potential to the rate of step motion is obtained by substituting Eqs. (20) and (21) into Eqs. (15), (16), and (10),

$$\frac{dx_i}{dt} = -\frac{D_s \Omega h_0 n_s^e \beta (x_i - x_{i-1})}{d_+(1+\beta) k_B T} \times \frac{\partial}{\partial x}\left\{\left(\frac{\partial h}{\partial x}\right)^{-1}\left[\frac{\partial}{\partial x}(\Delta\mu(x_i))\right]\right\}. \quad (22)$$

It can be seen from Eq. (22) that the rate of relaxation of a nonequilibrium configuration of steps towards an ideal equidistant configuration (having a zero contribution of the step-step repulsion to the chemical potential) is low when the parameter β is small, i.e., when the ES barrier is high. This is easy to understand since the relaxation of the step configuration takes place by detachment of atoms from those steps with high chemical potential, and their subsequent attachment to other steps with low chemical potential. These atoms must overcome the ES barrier either in the detachment, or in the attachment process.

Substituting the expression (22) into the equation

$$\frac{\partial h}{\partial t} = -h_0 \frac{dx_i/dt}{x_i - x_{i-1}} \quad (23)$$

used by Frank[43] in developing the kinematic theory of crystal growth, one obtains

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left\{\sigma\left[\frac{\partial}{\partial x}(\Delta\mu(x))\right]\right\}, \quad (24)$$

where

$$\sigma = \frac{D_s \Omega h_0^2 n_s^e \beta}{d_+(1+\beta) k_B T}\left(\frac{\partial h}{\partial x}\right)^{-1} \quad (25)$$

is a surface mobility relating the mass current in the curly brackets on the right-hand side of (24) to the gradient of the chemical potential $\Delta\mu$. The proportionality of the mobility (25) to the inverse of the surface slope is intimately related[44,45] to our assumption of a large kinetic length (slow detachment/attachment), i.e., case (b) [Eq. (14)]. Indeed, carrying out the same manipulations for the opposite case (a) [Eq. (13)], one arrives instead at the expression

$$\sigma = \frac{D_s \Omega h_0 n_s^e \beta}{k_B T[\beta + (d_+/\lambda_s)^2]} \quad (26)$$

which is independent of the surface slope.

Since the continuum limit of the expression (8) is[46]

$$\Delta\mu = -\frac{6\Omega A(T)}{h_0^2}\frac{\partial h}{\partial x}\frac{\partial^2 h}{\partial x^2}, \tag{27}$$

Eq. (24) can be presented as

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left\{ C\left(\frac{\partial h}{\partial x}\right)^{-1}\left[\frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\frac{\partial^2 h}{\partial x^2}\right)\right]\right\} = 0, \tag{28}$$

where

$$C = \frac{6A(T)D_s\Omega^2 n_s^e \beta}{d_+(1+\beta)k_BT} = \frac{3l_0^3\Omega D_s n_s^e\beta}{d_+(1+\beta)}. \tag{29}$$

A similar equation for the relaxation of the step bunches has been published previously.[45] It describes the relaxation of the fluctuations in the step density due to the step-step repulsion. Equation (28) is highly nonlinear and differs qualitatively from the linear evolution equation originally introduced by Mullins[47] to describe the relaxation of a crystal surface above the roughening temperature.

V. CONTINUUM THEORY OF BUNCH SHAPES

A. The continuum evolution equation

It was shown in Ref. 42 how the continuum limit for a set of step equations of the linear form (17) can be carried out in an essentially rigorous manner. The main idea is to perform the coarse graining operation on the level of the linear step dynamics, where it can be done exactly, and subsequently derive the evolution equation for the height profile $h(x,t)$ through a nonlinear variable transformation. Combining the result of this procedure with the continuum limit (28) for the relaxational dynamics, we obtain the full evolution equation for our problem. It takes the form of a continuity equation,

$$\frac{\partial h}{\partial t} + \frac{\partial J}{\partial x} = -h_0\hat{R}_e, \tag{30}$$

where the expression for the current is

$$J = -\frac{\hat{R}_e h_0^2(1-\beta)}{2(1+\beta)}\frac{1}{m} - \frac{\hat{R}_e h_0^3}{6}\frac{1}{m^3}\frac{\partial m}{\partial x} + \frac{C}{2}\frac{1}{m}\frac{\partial^2}{\partial x^2}m^2. \tag{31}$$

Here $m=\partial h/\partial x$ is the surface slope, which will be taken to be positive. The first term on the right-hand side of (31) is the destabilizing, downhill current which is responsible for the step bunching instability, while the last term describes the smoothing effect of the step-step repulsion, as described above. The second term is the only one to break the reflection symmetry ($x\to -x$ and $m\to -m$) of the evolution equation. As will be shown later, this term leads to different behavior at the upper and the lower edges of the bunch. Following earlier work,[42,48] we will refer to it as the symmetry-breaking term.

It is noteworthy that the continuum equation (30) conserves the volume of the film, apart from the constant sublimation rate on the right-hand side, which does not couple to the surface morphology. A dependence of the sublimation rate on the surface slope will be felt when the step spacing becomes comparable to the diffusion length.[37] In this sense Eq. (30) is valid only to leading order in l/λ_s.

B. Linear stability analysis

It is straightforward to derive from (30) and (31) the instability condition for a vicinal surface of slope $m_0=h_0/l$. We set $h(x,t)=m_0x-\hat{R}_e h_0 t+\epsilon_q(x,t)$, where $\epsilon_q(x,t)\sim e^{iqx+\omega(q)t}$ is a perturbation of wave number q, and expand (30) and (31) to linear order in ϵ. This yields the expression

$$\omega(q) = \frac{\hat{R}_e h_0^2(1-\beta)}{2(1+\beta)m_0^2}q^2 - Cq^4 - \frac{\hat{R}_e h_0^3}{6m_0^3}iq^3 \tag{32}$$

for the growth rate of the perturbation. The perturbation grows when $\mathrm{Re}(\omega)>0$, i.e., for wave numbers $q<q_{\max} = \sqrt{\hat{R}_e h_0^2(1-\beta)/[2(1+\beta)m_0^2 C]}$, and perturbations with wave number $q^*=q_{\max}/\sqrt{2}$ are maximally amplified. The corresponding wavelength is

$$\lambda^* = \frac{2\pi}{q^*} = 4\pi\sqrt{3S}l, \tag{33}$$

where we have introduced the dimensionless quantity

$$S = \frac{\beta}{1-\beta}\frac{\lambda_s^2 l_0^3}{d_+ l^4} = \frac{K_+K_-}{K_+-K_-}\frac{\tau}{l}\left(\frac{l_0}{l}\right)^3. \tag{34}$$

We will see below that the physical parameters of the problem enter the properties of the bunch shape only in the combination (34). It is interesting to note that S does not depend on the surface diffusion constant D_s. The wavelength λ^* determines the linear size of bunches in the beginning of the bunching instability. Correspondingly the number of steps in an incipient bunch is given by

$$N^* = \lambda^*/l = 4\pi\sqrt{3S} \approx 21.8\times\sqrt{S}. \tag{35}$$

The imaginary part of the growth rate (32), which derives from the symmetry-breaking term in (31), does not affect the stability of the surface, but it induces a drift of fluctuations.

C. The mechanical analog

Our main goal in this section is to compute the shape of large, almost stationary bunches from Eq. (31). For a stationary profile, the current (31) is set to a constant J_0. We neglect the symmetry-breaking term for now, and return to its relevance at the end of the section. Introducing the quantity $u=m^2$, which is positive by construction, the stationarity condition $J\equiv J_0$ can then be written in the familiar form

$$\frac{C}{2}\frac{d^2u}{dx^2} = B + J_0u^{1/2} = -\frac{dV}{du} \tag{36}$$

of a classical particle coordinate $u(x)$ moving in a potential $V(u)=-Bu-(2/3)J_0u^{3/2}$, where $B=\hat{R}_e h_0^2(1-\beta)/[2(1+\beta)] >0$ and J_0 must be chosen negative. The bunch is a particle trajectory which starts at $u=0$ at "time" $x=0$, reaches a turning point $u=u_{\max}$ at time $x=L/2$, and returns to $u=0$ at time $x=L$. Here L can be identified with the bunch width, and the

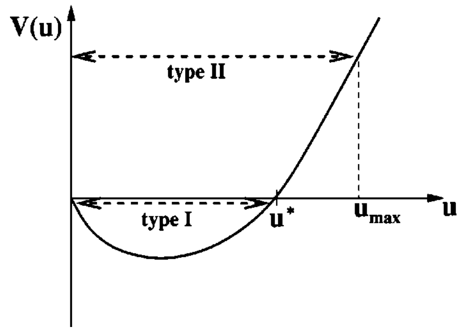

FIG. 2. Sketch of the potential $V(u)$ appearing in the mechanical analog. The dashed arrows illustrate trajectories of type I and type II.

minimal terrace length in the bunch introduced previously is given by $l_{\min}=h_0/\sqrt{u_{\max}}$.

As can be seen in Fig. 2, the potential $V(u)$ admits two types of periodic trajectories. When the total particle "energy" $\mathcal{E}=(C/4)(du/dx)^2+V(u)$ is negative, u performs an essentially harmonic motion around the minimum of the potential. This will be referred to as a type I solution. The particle velocity du/dx vanishes at both turning points, which translates into the vanishing of the curvature dm/dx of the surface profile. The height profile represented by such a trajectory is a periodic array of step bunches which is everywhere smooth. In contrast, particle trajectories with positive total energy (type II solutions) reach the reflecting "hard wall" at $u=0$ at a finite speed. This implies that the surface curvature $dm/dx=(du/dx)/2m$ diverges as $m\to 0$, such that the surface profile develops singularities of the type

$$h(x)-h(x_0)\sim(x-x_0)^{3/2} \tag{37}$$

near the bunch edges at $x=x_0$. This is the well-known Pokrovsky-Talapov law which describes how the rounded parts of an equilibrium crystal shape join a flat facet,[35] and is reflected in the scaling of the terrace sizes at the edges of the bunch (see Sec. V E). Because of the singularities at the bunch edges, type II height profiles have finite support and cannot be continued to describe a periodic array of bunches.

We now show that the two types of trajectories imply different scaling properties for the step bunches. For a trajectory of type I to satisfy the boundary conditions $u(0)=u(L)=0$ for $L\to\infty$, it is necessary to set the particle energy $\mathcal{E}=0$. The right turning point is then located at the value $u^*=(3B/2J_0)^2$ at which $V(u^*)=0$, and the period of the trajectory is readily seen to be of the order of $L\sim\sqrt{BC}/|J_0|$. Bunches of arbitrary (large) lateral size L can therefore be accommodated only by treating J_0 as a free integration constant, and to let $J_0\sim 1/L\to 0$ for $L\to\infty$. This is the procedure adopted in Ref. 34 for a slightly different case. In the present context it implies the scaling relation $l_{\min}\sim 1/\sqrt{u^*}\sim|J_0|\sim 1/L$, and since the number of steps in the bunch is of the order $N\sim L/l_{\min}$, we find that $l_{\min}\sim N^{-1/2}$. For future reference we record the full expressions for L and $l_{\min}$, which read

$$L=(216S)^{1/4}N^{1/2}l,\quad l_{\min}=\frac{2}{3}\frac{L}{N}=\left(\frac{128S}{3}\right)^{1/4}\frac{l}{N^{1/2}}. \tag{38}$$

For type II trajectories with $\mathcal{E}>0$, it is possible to make the period arbitrarily large while keeping J_0 fixed, simply by increasing the energy. For large bunches we then have $u_{\max}\gg u^*$, and the decreasing part of the potential becomes irrelevant. The equation for the profile reduces to the form

$$C\frac{d}{dx}\left(m\frac{dm}{dx}\right)=-|J_0|m, \tag{39}$$

which was first studied by Noziéres,[44] and leads to the scaling law[24,29,44] $l_{\min}\sim N^{-2/3}$ (see Sec. V E for a detailed derivation). Anticipating the results of the numerical solution of the discrete step equations in Sec. VII, it turns out that this scaling law is in agreement with the numerical data for $l_{\min}$, while the prediction (38) for type I trajectories is not. We conclude, therefore, that the type II trajectories of (36), with singular behavior at $u=0$, are the relevant solutions for the description of step bunches. This immediately raises the question of how the current J_0, which then no longer can be treated as an integration constant, should be determined. The answer will be given in the next section.

We add a final remark comparing the two types of solutions. On purely mathematical grounds, at first sight the type I solutions may seem to be preferable, because they avoid the singularities at the bunch edges and allow to describe a periodic array of many bunches. This is in fact not the case. For a periodic type I profile, the end of one bunch (the point where $m=u=0$) defines the beginning of the next. As, according to (38), the bunches steepen with increasing size, the mean slope of the surface also increases without bound. This is in contradiction to the time evolution of a real surface, for which the mean slope is fixed and the steepening of the bunches is compensated by the growth of large flat regions between the bunches (see Fig. 1). For type I solutions, the region between bunches shrinks to a point. Therefore they cannot be taken at face value as a global description of a surface with many bunches. Just like for the type II solutions, which terminate in singularities, also type I solutions must be complemented by a separate description for the flat regions between bunches.

D. The mean surface current

Our strategy will be to determine J_0 by analogy with two related problems, which are mathematically equivalent to the present one (see Sec. VI for further discussion). The two problems are the linear step growth model considered in Ref. 42, and the model of surface electromigration in the attachment/detachment-limited regime considered in Ref. 24. Indeed, the step equations derived by Liu and Weeks[24] for surface electromigration in the presence of desorption but without Ehrlich-Schwoebel barriers are (apart from the different physical meaning of the coefficients) identical to our equations (17). By appealing to the analogy with surface electromigration, we can associate a microscopic current j_i with the terrace between the steps i and $i+1$, which is given by the expression

$$j_i = -h_0\hat{D}[\Delta\mu(x_{i+1}) - \Delta\mu(x_i)] - \frac{(1-\beta)}{2(1+\beta)}h_0\hat{R}_e(x_{i+1}-x_i). \tag{40}$$

Here the abbreviation $\hat{D}=D_s\Omega n_s^e\beta/[d_+k_BT(1+\beta)]$ has been introduced. The physical meaning of this current is clear in the context of surface electromigration—it is simply the current of adatoms driven across the terrace by the combined action of the electromigration force and the chemical potential gradient. The notion of a surface current induced by attachment asymmetry is also well established in the context of epitaxial growth.[40,42,49–51] It is less evident that the concept can be extended to sublimation, where the atoms detached from the steps do not necessarily remain on the terrace. However, as was noted above in Sec. V A, we are working here in a limit where the diffusion length λ_s is very large, and hence the mass transport is essentially confined to the surface. Mathematically, the derivation in Ref. 42 shows that for a general set of step equations which are linear in the terrace widths,

$$\frac{dx_i}{dt} = \gamma_-(x_{i+1}-x_i) + \gamma_+(x_i - x_{i-1}), \tag{41}$$

the leading order (stabilizing or destabilizing) part of the surface current is proportional to the asymmetric combination $\gamma_- - \gamma_+$ of the contributions from the two terraces, while the symmetric combination $\gamma_- + \gamma_+$ gives rise to the overall growth (or sublimation) rate of the surface, and to the symmetry-breaking part of the surface current.

For a perfect step train with constant step spacing l, the current (40) is equal to

$$J_{\mathrm{flat}} = -\frac{1-\beta}{2(1+\beta)}h_0\hat{R}_e l, \tag{42}$$

which is just the first term in (31) evaluated at slope $m=h_0/l$. Following Liu and Weeks,[24] we now argue that the expression (42) remains valid also for a periodic array of step bunches. Each bunch contains N steps, and hence consists of $N-1$ short terraces. The width of each bunch is L, and the bunches are separated by terraces of length L_t. We denote by $\Delta\mu_-$ and $\Delta\mu_+$ the values of the chemical potential at the lower and upper edges of the bunch. Summing the expression (40) across the bunch, we find that the current in the bunch is equal to

$$j_b = -\frac{h_0}{N-1}\left[\hat{D}(\Delta\mu_+ - \Delta\mu_-) + \frac{(1-\beta)}{2(1+\beta)}\hat{R}_e L\right], \tag{43}$$

while the current on the terrace is

$$j_t = -h_0\hat{D}(\Delta\mu_- - \Delta\mu_+) - \frac{(1-\beta)}{2(1+\beta)}h_0\hat{R}_e L_t. \tag{44}$$

Stationarity requires that $j_b=j_t$, which yields an expression for the chemical potential difference $\Delta\mu_+ - \Delta\mu_-$. Inserting this back into (43) or (44), we find the simple result

$$j_b = j_t = -\frac{(1-\beta)}{2(1+\beta)}h_0\hat{R}_e\frac{L+L_t}{N}, \tag{45}$$

which coincides with (42). Thus the overall current remains constant, at its value for a regular step train, throughout the bunching process, and the appropriate expression to use for J_0 in (36) or (39) is J_{flat}.

It is possible to argue for this choice of J_0 also without reference to the discrete step dynamics. Indeed, setting $J_0=J_{\mathrm{flat}}$ ensures that the minimum of the potential $V(u)$ is located at the value $u=(h_0/l)^2$ corresponding to the mean surface slope. In this way the initial regular step train, which is clearly an (unstable) stationary solution of the discrete step dynamics, is retained as a solution also in the stationary continuum equation.

E. Derivation of the scaling laws

The solution of the mechanical problem (36) allows to express the bunch width L and the bunch height H in terms of the maximal slope $m_{\max}=\sqrt{u_{\max}}$. Using energy conservation and neglecting the linear term $-Bu$ in the potential $V(u)$, we obtain the expressions

$$L = \sqrt{\frac{3C}{2|J_0|}}\int_0^{u_{\max}}\frac{du}{\sqrt{u_{\max}^{3/2}-u^{3/2}}} \approx 2.11\sqrt{\frac{C}{|J_0|}}m_{\max}^{1/2} \tag{46}$$

and

$$H = \sqrt{\frac{3C}{2|J_0|}}\int_0^{u_{\max}}\frac{\sqrt{u}du}{\sqrt{u_{\max}^{3/2}-u^{3/2}}} = \sqrt{\frac{8}{3}}\sqrt{\frac{C}{|J_0|}}m_{\max}^{3/2}. \tag{47}$$

The dimensionless coefficient in (46) was obtained by numerically evaluating the corresponding integral. Inserting the expressions (29) and (42) for C and J_0, respectively, we can write the minimal terrace length $l_{\min}$ and the bunch width L in terms of the number of steps and dimensionless ratios of length scales, as

$$\frac{l_{\min}}{l} = 2^{4/3}\left(\frac{\beta}{1-\beta}\right)^{1/3}\left(\frac{l}{d_+}\right)^{1/3}\left(\frac{\lambda_s}{l}\right)^{2/3}\left(\frac{l_0}{l}\right)N^{-2/3} = 2^{4/3}S^{1/3}N^{-2/3} \tag{48}$$

and

$$\frac{L}{l} \approx 3.25\left(\frac{\beta}{1-\beta}\right)^{1/3}\left(\frac{l}{d_+}\right)^{1/3}\left(\frac{\lambda_s}{l}\right)^{2/3}\left(\frac{l_0}{l}\right)N^{1/3} = 3.25S^{1/3}N^{1/3}. \tag{49}$$

Equations (48) and (49) are the central results of this section, and will be compared to numerical simulations of the discrete step model in Sec. VII. Together (48) and (49) imply the universal relation $L/l_{\min}\approx 1.29N$, independent of all physical parameters. This shows that the minimal terrace length is only a factor 0.78 smaller than the mean terrace length L/N within the bunch, hence most terraces in the bunch have a size of order $l_{\min}$.

A separate scaling law holds for the size of the first (and last) terrace at the edges of the bunch. To derive it, we need to determine the precise bunch profile near $u=0$, which is of the general form (37). Since the mechanical potential $V(u)$ vanishes at $u=0$, energy conservation implies that $(C/4)\times(du/dx)^2=\mathcal{E}=V(u_{\max})$ for $u\to 0$. Integrating this from the bunch edge at $x=0$ yields the slope profile $m(x)=(4\mathcal{E}/C)^{1/4}x^{1/2}$, and correspondingly the height profile $h(x)=(2/3)(4\mathcal{E}/C)^{1/4}x^{3/2}$. There is an ambiguity in how to estimate the size l_1 of the first terrace—a quantity manifestly related to the discreteness of the surface in the vertical direction—from these continuous profiles. Natural choices would be to require that (i) $h(x=l_1)=h_0$, (ii) $m(x=l_1)=h_0/l_1$ or (iii) $m(h=h_0)=h_0/l_1$. It is easy to check that all three choices imply a scaling relation of the form $l_1\sim S^{1/3}N^{-1/3}$, but with different numerical coefficients. Because the continuum equation is derived[42] from a set of discrete equations for the terrace sizes (the inverse slopes) as a function of the layer height, we claim (and confirm numerically in Sec. VII) that choice (iii) is the appropriate one. This results in

$$\frac{l_1}{l}=4^{1/3}\left(\frac{\beta}{1-\beta}\right)^{1/3}\left(\frac{\lambda_s}{l}\right)^{2/3}\left(\frac{l}{d_+}\right)^{1/3}\left(\frac{l_0}{l}\right)N^{-1/3}=4^{1/3}S^{1/3}N^{-1/3}. \tag{50}$$

The same kind of analysis can be carried out for the type I solutions discussed in Sec. V C. One finds that $l_1/l\sim S^{1/4}$ independent of the bunch size N.

F. General step interaction

The above considerations are easily generalized to different values for the exponent n describing the decay of the step-step interaction as $1/l^n$. The expression (8) for the chemical potential at step i then becomes

$$\frac{\Delta\mu(x_i)}{k_BT}=-\left(\frac{l_0}{x_{i+1}-x_i}\right)^{n+1}+\left(\frac{l_0}{x_i-x_{i-1}}\right)^{n+1} \tag{51}$$

with $l_0=(n\Omega A/k_BT)^{1/(n+1)}$, and going through the manipulations of Sec. IV one obtains the generalized relaxation equation

$$\frac{\partial h}{\partial t}+\frac{\partial}{\partial x}\left\{C_n\left(\frac{\partial h}{\partial x}\right)^{-1}\left[\frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\right)^{n-1}\frac{\partial^2 h}{\partial x^2}\right]\right\}=0 \tag{52}$$

with

$$C_n=\frac{(n+1)l_0^{n+1}\Omega D_s n_s^e\beta h_0^{2-n}}{d_+(1+\beta)}. \tag{53}$$

The analysis of the resulting full continuum equation leads to the scaling relations[26]

$$l_{\min}\sim N^{-2/(n+1)},\quad L\sim N^{(n-1)/(n+1)},\quad l_1\sim N^{-1/(n+1)} \tag{54}$$

for type II solutions. Specifically, the relations (48) and (50) generalize to

$$l_{\min}/l=(16S_n)^{1/(n+1)}N^{-2/(n+1)}=(16S_n/N^2)^{1/(n+1)},$$
$$l_1/l=(4S_n/N)^{1/(n+1)}, \tag{55}$$

where the dimensionless parameter S_n is defined by

$$S_n=\frac{\beta}{1-\beta}\frac{\lambda_s^2 l_0^{n+1}}{dl^{n+2}}=\frac{K_+K_-}{K_+-K_-}\frac{\tau}{l}\left(\frac{l_0}{l}\right)^{n+1}. \tag{56}$$

Comparing the two expressions in (55) it is seen that $l_{\min}$ becomes smaller than l_1 only for $N>4$; this can be viewed as a necessary condition for the onset of scaling. If we require in addition that $l_1/l<1$, it follows that such small bunches can form only provided $S_n<1$.

For type I solutions the scaling relations corresponding to (54) read

$$L\sim S_n^{1/(n+2)}N^{n/(n+2)},\quad l_{\min}\sim S_n^{1/(n+2)}N^{-2/(n+2)}. \tag{57}$$

G. Corrections to the asymptotic behavior

The scaling laws derived in the preceding section are valid asymptotically for large bunches, when the two approximations made in their derivation are well justified: First, neglecting the symmetry-breaking contribution to the current (31), and second, neglecting the constant term in the particle equation (36). The second approximation is valid provided $u_{\max}\gg u^*$, where $u^*=(3B/2J_0)^2$ is the value of u at which $V(u^*)=0$. Inserting the expression (42) for J_0, we see that the corresponding slope $m^*=\sqrt{u^*}$ is simply of the order of the mean slope h_0/l of the surface. Thus the linear term in $V(u)$ can be ignored throughout the bunch.

Including the symmetry-breaking term, the stationarity condition $J=J_0$ can be brought into the form

$$S\frac{d^2v}{dy^2}=\frac{1}{3}(1-\sqrt{v})+\frac{1+\beta}{18(1-\beta)}\frac{1}{v^{3/2}}\frac{dv}{dy}, \tag{58}$$

where $v=(l/h_0)^2u$ is a dimensionless version of u, normalized such that the mean slope corresponds to $v=1$, and $y=x/l$ is the dimensionless spatial coordinate. In the mechanical analog of Sec. V C, the symmetry-breaking term corresponds to a friction force which, because of its sign, acts "backward" in time. The friction force is proportional to $v^{-3/2}$. Hence it is negligible deep inside the bunch, where $v\gg 1$, but becomes important near the edges of the bunch.

It is instructive to follow the solution of Eq. (58) starting from the center of the bunch, where $v(y)$ takes its maximum value $v_{\max}$ and $dv/dy=0$. Integrating forward in "time" y, towards the upper edge of the bunch, the friction force adds to the acceleration of the particle towards $v=0$, which is therefore reached earlier than in the absence of the symmetry-breaking term. Moreover the singular behavior at $v=0$ is altered: Balancing the symmetry-breaking term against the inertial term on the left-hand side of (58), it is straightforward to show that the standard behavior (37) of the height profile is modified into

$$h(x_0)-h(x)\sim(x_0-x)^{4/3}. \tag{59}$$

Conversely, when moving backward in time (towards the lower edge of the bunch) the particle is delayed by the fric-

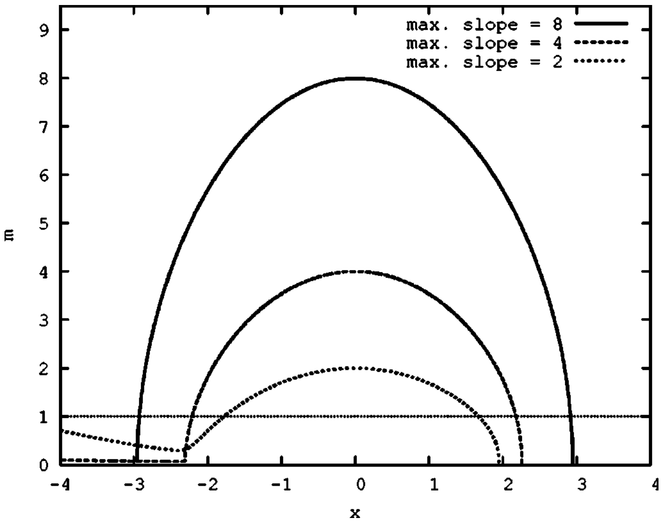

FIG. 3. Stationary bunch shapes computed by numerical integration of Eq. (58) with $S=0.14$ and $\beta=0.01$. The figure shows the dimensionless slope $(l/h_0)m(x)$ as a function of the rescaled coordinate x/l for different values of the maximum slope. The horizontal dotted line shows the value $m=h_0/l$ corresponding to the mean slope of the unperturbed surface.

tion force. Since the friction coefficient diverges as $v\to 0$, the point $v=0$ is never reached. Instead, the trajectory bounces back and approaches the stable potential minimum at $v=1$ in an overdamped or damped oscillatory manner. Since the parameter S plays the role of the particle mass in (58), the effects of friction increase with decreasing S, while they decrease when increasing the initial particle energy (i.e., the value of $v_{\max}$, and, hence, the size of the bunch).

Thus the symmetry-breaking term modifies the nature of the solutions of (58) in a qualitative way: Whereas the relevant solutions of the frictionless particle problem (36) have finite support in x (the trajectory returns to $u=0$ in a finite time), the solutions of (58) extend all the way to $y=-\infty$, where v attains the limiting value $v=1$. In physical terms this implies that the bunch width L can no longer be sharply defined within the continuum theory. Nevertheless, the numerical solutions of (58) depicted in Fig. 3 show that this effect is completely negligible already for moderately large bunches and physically relevant values of S. Deviations from the solution of the frictionless equation (36) occur only in the range $v \ll 1$, which is irrelevant for the description of actual bunches (recall that $v=1$ corresponds to the mean slope h_0/l of the unperturbed surface). This conclusion is supported by a scaling analysis in the spirit of Ref. 36 (see Sec. VIII).

We will see in Sec. VII that the left-right symmetry of the bunches is indeed broken in a way that is qualitatively reminiscent of the solutions of (58) with very small S. However, the sign of the observed symmetry-breaking is opposite to that predicted by (58), and we will argue that its origin is in fact completely different.

VI. EQUIVALENT PROBLEMS

We noted already in Sec. V D that the equations of step motion (10), (15), and (16) are mathematically equivalent to appropriate limiting cases of those obtained for step bunching instabilities induced by electromigration and growth in the presence of inverse Ehrlich-Schwoebel barriers. Here we elaborate on that observation and translate the results derived from the continuum theory to the different physical contexts.

A. Electromigration

Discrete and continuum equations for electromigration-induced step bunching in the attachment/detachment limited regime have been derived by Liu and Weeks,[24] and their equations are readily seen to be of the same form as ours. In our setting, an electromigration force F acting on the adatoms can simply be added to the chemical potential gradient on the right-hand side of (24). This gives rise to an additional contribution $J_F=\sigma F$ to the surface current J in (30), which is also inversely proportional to the slope m [see the expression (25) for σ in the attachment/detachment limited case], and which is destabilizing for $F<0$ (force in the downhill direction). In the absence of an Ehrlich-Schwoebel effect ($\beta=1$), the electromigration current is the only destabilizing contribution. The results of Sec. V carry directly over to this case, once the dimensionless parameter S has been identified along the lines of Sec. V B. One finds the simple result

$$S=\frac{\Omega A}{Fl^4} \tag{60}$$

and hence from (48)–(50) we obtain the predictions

$$l_{\min}=\left(\frac{16\Omega A}{Fl}\right)^{1/3}N^{-2/3},$$
$$L\approx 3.25\left(\frac{\Omega A}{Fl}\right)^{1/3}N^{1/3},$$
$$l_1=\left(\frac{4\Omega A}{Fl}\right)^{1/3}N^{-1/3}. \tag{61}$$

Similar formulas have been reported previously in the literature. Sato and Uwaha derived the results[26]

$$L/N\approx 2.59\left(\frac{\Omega A}{Fd}\right)^{1/3}N^{-2/3},$$
$$l_{\min}=\left(\frac{8\Omega A}{Fd}\right)^{1/3}N^{-2/3},$$
$$l_1=\left(\frac{2\Omega A}{Fd}\right)^{1/3}N^{-1/3}, \tag{62}$$

which are of the same form as the expressions in (61), with the kinetic length $d=d_-=d_+$ replacing the mean step spacing l. This reflects the fact that Sato and Uwaha work in the diffusion-limited regime $d<l$.

Stoyanov and Tonchev[29] have developed a continuum description for electromigration-induced step bunching in the diffusion-limited regime. Assuming the relation $d=a_\parallel$ for the kinetic length, which holds for nonpermeable steps in the absence of an additional barrier against attachment, they obtained the evolution equation

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left[\tilde{B}m + \frac{\tilde{C}}{2}\frac{\partial^2}{\partial x^2}m^2\right] = 0, \tag{63}$$

where $m = \partial h / \partial x$ is the surface slope, and the coefficients $\tilde{B}$ and $\tilde{C}$ are given by

$$\tilde{B} = -\frac{2D_s n_s^e F \Omega a_\perp}{k_B T}, \quad \tilde{C} = \frac{6D_s n_s^e \Omega^2 A}{h_0 k_B T}. \tag{64}$$

The surface is unstable when the force is in the downhill direction, $F<0$ and $\tilde{B}>0$. The relaxation term in (63) is simply the product of the chemical potential variation (27) and the expression (26) for the mobility in the diffusion-limited case, where it has been used that $d_+ \ll \lambda_s$ and $\beta = 1$.

The analysis of stationary solutions of (63) proceeds along the lines of Sec. V C. In fact, the mechanical analog resulting from setting the square brackets in (63) equal to a constant current $\tilde{J}_0$ is formally identical to (36), with the potential $V(u) = -\tilde{J}_0 u + \tilde{B}u^{3/2}$. Despite the formal similarity, however, the problem differs from that considered in Sec. V C in one important respect: Since the overall surface current is downhill, we must choose $\tilde{J}_0 < 0$, and hence both terms in the potential are positive; the potential has no minimum, and type I trajectories do not exist. For the type II trajectories the term proportional to $\tilde{J}_0$ becomes irrelevant at large slopes, and hence one may as well set $\tilde{J}_0 = 0$, as was done in Ref. 29. The bunch shape is then given by the solution of (39), and the results of Sec. V E can be taken over. This yields the scaling relations

$$L/N \approx 2.58\left(\frac{a_\parallel A}{F}\right)^{1/3} N^{-2/3},$$

$$l_{\min} = 2\left(\frac{a_\parallel A}{F}\right)^{1/3} N^{-2/3}. \tag{65}$$

Apart from a small difference in the dimensionless prefactor, the expression for L/N is identical to the one reported in Ref. 29.

Relations of the form (65) have been used in the interpretation of several experiments on silicon surfaces, where a scaling of the minimal terrace size[31] and the mean terrace size[32] as $N^{-2/3}$ was observed. The similarity between the expressions (61), (62), and (65) implies that it is not possible to distinguish between attachment/detachment limited kinetics and diffusion-limited kinetics on the basis of the observed scaling; see Sec. VIII for further elucidation of this point. However, the resulting estimate for the ratio A/F depends crucially on which kinetic regime is assumed. Consider, for example, the results obtained by Fujita, Ichikawa, and Stoyanov[31] for the maximum bunch slope $h_0/l_{\min}$ at 1250 °C. Using the relation (65) for the diffusion-limited regime yields the estimate $F/A \approx 3 \times 10^{-6}\ \mathrm{nm}^{-2}$; this is somewhat larger than the value reported in Ref. 31, because in that work the authors used an expression for the mean terrace width $\bar{l} = L/N$. Because of the additional factor of l, application of (61) yields instead $F/A \approx 6 \times 10^{-8}\ \mathrm{nm}^{-2}$, which is smaller by a factor of 50. Correspondingly the effective valence Z^* of the silicon adatoms, defined through the relation $F = Z^* eE$ between the electromigration force and the electric field E, will be smaller by the same factor.

B. Growth with inverse Ehrlich-Schwoebel barriers

Growth in the presence of an inverse Ehrlich-Schwoebel effect is described by the stationary diffusion equation (5) with $R>0$ and $1/\tau_s = 0$, and the boundary conditions (6) with $K_- > K_+$, i.e., $\beta > 1$. While the possibility of inverse ES barriers is debatable on the microscopic level, the inverse ES effect may serve as a useful effective description of more complex step bunching mechanisms.[52] The equations of step motion can be found, e.g., in Ref. 12. We consider the limiting case of fast attachment to the descending step and slow attachment to the ascending step, i.e., $d_+ \gg x_i - x_{i-1} \gg d_-$. In this limit only the upper terrace contributes to the growth of the step, and the destabilizing part of the dynamics reduces to the linear form (41) with $\gamma_+ = 0$ and $\gamma_- = -R\Omega$ (note that in our setup the steps recede during growth and the upper terrace trails the step). The continuum equation is thus of the same form as in sublimation and electromigration, and the results of Sec. V carry over with the identification

$$S = \frac{D_s n_s^e l_0^3}{R d_+ l^4} \tag{66}$$

of the dimensionless parameter. The application of the continuum theory to this problem will be the subject of a separate publication.[14]

VII. NUMERICAL ANALYSIS OF THE DISCRETE STEP DYNAMICS

Extensive numerical simulations of the discrete step dynamics have been carried out to test the predictions of the continuum theory. In this section we report on simulations for the sublimation problem; a comprehensive numerical study of growth in the presence of an inverse Ehrlich-Schwoebel effect will be presented elsewhere.[14] We work with cyclic boundary conditions, $x_{M+1} = x_1 + Ml$ where l is the average interstep distance of the vicinal surface and M is the total number of steps, and prepare the system in one of two kinds of initial conditions. Under *natural bunching conditions*, the integration is started from a vicinal surface with steps which slightly deviate from their regular positions. This leads to a surface consisting of many bunches of steps separated by large terraces, which slowly coarsens (Fig. 4). On the other hand, a *single bunch* can be prepared by chosing an initial step configuration, corresponding to a bunch, which contains almost all of the steps in the system. The integration then provides results for the steady state shape of the bunch and the average value of the number N of steps in it (the remaining $M-N$ steps are single—they are crossing the large terrace between the front edge of the bunch and its tail in our single bunch setup with cyclic boundary conditions). In both cases we assume that a given step belongs to the bunch when the distance to at least one of the neighboring steps is smaller than 0.75 l. This definition is, in fact, arbitrary and it introduces some ambiguity in the results. The dependence of the

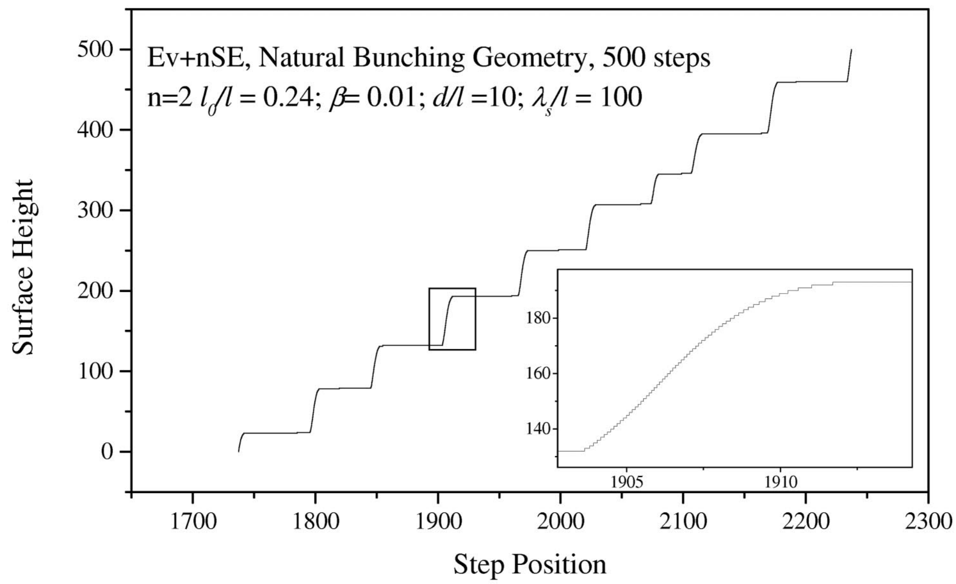

FIG. 4. Profile of a crystal surface after some time of sublimation, with dimensionless parameters $l_0/l=0.24$, $\beta=0.01$, $d_+/l=10$, and $\lambda_s/l=100$. The inset shows the enlargement of an individual bunch.

minimum distance $l_{\min}$ between the steps in the bunch on the number N of steps is less affected by this ambiguity than that of the total bunch width L, as in the former case only N is influenced by the definition, whereas $l_{\min}$ is precisely determined.

We first present results from the numerical integration of the sublimation problem in case (b) of Sec. III, i.e., (10) was used with v_- and v_+ given by (15) and (16), with the destabilizing terms depending linearly on the terrace widths. The equations of step motion contain four dimensionless parameters, λ_s/l, d_+/l, l_0/l, and $\beta=K_-/K_+$. It is reasonable to briefly discuss the values of these parameters. For instance the value $\lambda_s/l=100$ means that $\lambda_s=1$ μm at $l=10$ nm. As far as the values of the parameter d_+/l are concerned, it is difficult[41] to evaluate the kinetic length d_+. We should have in mind, however, that Eqs. (15) and (16) are valid under the assumption $(x_i-x_{i-1})\ll d_+$ and, therefore, we must take $d_+/l \gg 1$. The value of the parameter l_0/l was assumed to be $l_0/l=0.24$ in order to keep the interstep distance in the bunch to be in a convenient interval. Finally, the values of β used were $\beta=0.01$ and $\beta=0.1$ corresponding to a rather high Ehrlich-Schwoebel barrier. Figure 5 shows four sets of data for $l_{\min}$ as a function of N obtained for two different step interaction laws, $n=2$ and $n=3$, using the natural bunching as well as the single bunch initial conditions. In all cases excellent agreement with the theoretical prediction (55) is found. The same quality of agreement has been obtained for the problem of growth with inverse Ehrlich-Schwoebel barriers.[14]

In Fig. 6 we show data for the dependence of the total bunch width L on the number of steps. Although the overall magnitude of L is consistent with the prediction (49) for type II stationary profiles (and rules out type I behavior), a power law fit to the data yields an estimate $\alpha\approx0.44$ which is intermediate between the type II ($\alpha=1/3$) and type I ($\alpha=1/2$) predictions. To gain some insight into this discrepancy, we take a closer look at the shapes of the bunches in the numerical simulation (Fig. 4). It is clear that the bunches are distinctly *asymmetric*: While there is an abrupt change in the terrace length at the lower (trailing) edge of the bunch, at the upper (leading) edge the terrace lengths increase gradually. The asymmetry can be quantified by looking at the scaling of the size of the first (l_1) and last (l_N) terrace in the bunch with the bunch size N (Fig. 7). While the data for l_1 are in good agreement with the theoretical prediction (55), the size of the last terrace is found to be essentially independent of N. Incidentally, the latter behavior is also characteristic of the type I stationary profiles (see Sec. V E). More significantly, a constant last terrace size $l_N\sim l$ results trivially from our way of numerically locating the bunch edge, if the terrace size increases continuously across the mean terrace size as one moves out of the bunch in the forward direction, i.e., if a sharply defined bunch edge in fact does not exist.

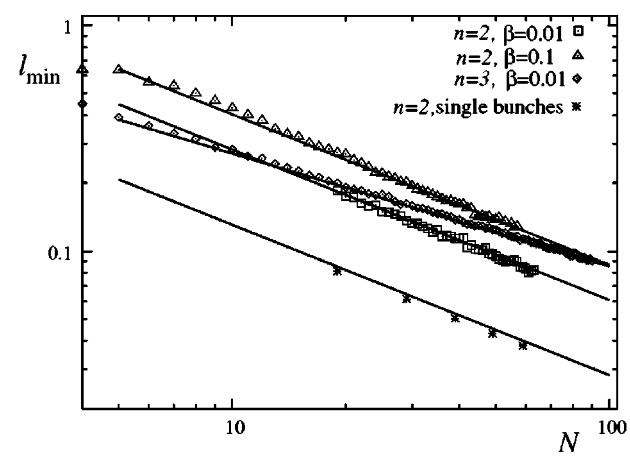

FIG. 5. Numerical data for the minimum interstep distance, measured in units of l, as a function of bunch size. Open symbols show results obtained in the natural bunching geometry with 500 steps, while asterisks show data obtained from computations with a single bunch. The interaction strength was $l_0/l=0.24$ in all cases. Open squares and diamonds show data for $d_+/l=10$ and $\lambda_s/l=100$, triangles show data for $d_+/l=150$ and $\lambda_s/l=200$, and asterisks show data for $d_+/l=\lambda_s/l=100$; other parameters are given in the figure. Bold lines show the theoretical prediction (55) for $l_{\min}$.

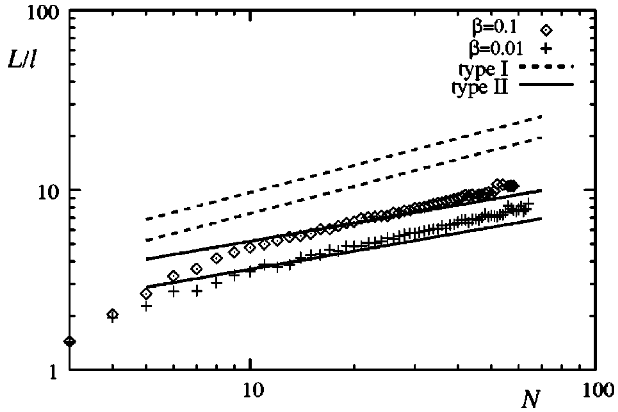

FIG. 6. Numerical results for the bunch width L as a function of bunch size. Data are shown for two of the parameter sets displayed in Fig. 5: $\beta=0.1$, $\lambda_s/l=200$, $d_+/l=150$ (diamonds), and $\beta=0.01$, $\lambda_s/l=100$, $d_+/l=10$ (crosses). In both cases $l_0/l=0.24$ and the system contained 500 steps. Dashed and full lines show the predictions for type I and type II solutions, respectively. A power law fit to the data yields $L\sim N^{0.44}$.

What is the origin of the asymmetry in the bunch shape? We have shown in Sec. V G that the symmetry-breaking term causes the bunch edge to fray out at one side, in a qualitatively similar manner to the behavior seen in Fig. 4. However, the blurring of the bunch edge is predicted to occur at the lower (trailing) edge, rather than at the upper edge, and in addition the effect becomes negligibly small already for moderately sized bunches (see Fig. 3). We believe, instead, that the bunch asymmetry is intimately related to the exchange of *crossing steps* between bunches. These steps gradually accelerate out of the bunch at the leading edge, which translates into a gradual increase of the mean terrace size. Conversely, when approaching the next bunch from behind, the crossing step decelerates quite abruptly, because it is primarily fed from behind (this is particularly true in the almost one-sided regime mainly considered in our simulations). The exchange of steps between bunches also implies that the bunches move laterally at a speed which is different from the mean sublimation rate. To capture the asymmetry in

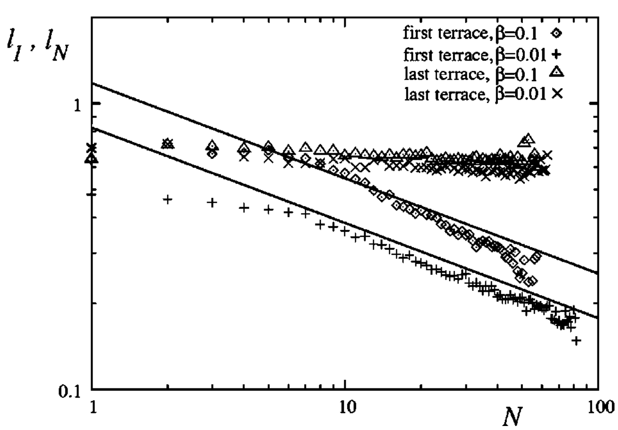

FIG. 7. Scaling of the first and last terrace size in the bunch with bunch size for the same parameter sets as in Fig. 6. The full lines show the theoretical prediction for type II solutions.

the continuum theory, it will therefore be necessary to go beyond the stationary solutions considered in Sec. V, which by construction are symmetric, and to investigate solutions describing moving and interacting bunches. It is worth pointing out that the existence of crossing steps partly invalidates the argument used in Sec. V D to fix the mean surface current, because the argument assumes that all steps reside in bunches.[24]

We close this section with some remarks concerning the limiting case (a) of Sec. III. We have shown that no bunching occurs in this case, i.e., when the assumption $x_i-x_{i-1}>d_+$ is fulfilled, if only the linear and quadratic terms $[(x_i-x_{i-1})/\lambda_s$ and $(x_i-x_{i-1})^2/\lambda_s^2]$ in the expressions for the step velocity are taken into account. To clarify the problem of step bunching instability in the limiting case (a) we did a lot of numerical work making use of the full expressions for the step velocity. Integration of the equations of step motion proved the existence of step bunching at parameter values $\beta=0.01$, $l_0/l=0.003$ and $d_+/l=1/3$, $d_+/l=1/30$, and $d_+/l=1/300$. It is essential to note, however, that the magnitude of the step-step repulsion energy used in these integration runs was much smaller than in the integration of the equations obtained in the case $d_+\gg l$, where we used $l_0/l=0.24$. On the other hand, the density of steps in the bunch is higher in the case $d_+\gg l$ compared with the opposite limiting case $d_+\ll l$. These findings indicate a strong impact of the parameter d_+ on the bunching process. When the parameter d_+ is larger than the interstep distance l, bunching occurs even at a very strong repulsion between the steps and the step density in the bunch is rather high. On the contrary, when the parameter d_+ is smaller than the interstep distance l, bunching occurs only at a very weak repulsion between the steps and the step density in the bunch is relatively small. This is not surprising because in the case under consideration neither the linear nor the quadratic term induces instability of the vicinal surface. Destablizing terms are of higher order, i.e., $[(x_i-x_{i-1})/\lambda_s]^\nu$ with $\nu>2$ and their effect is relatively weak so that it cannot dominate a strong repulsion between the steps. It is interesting to note, however, that in this case of weak instability $(d_+\ll l)$ the minimum interstep distance in the bunch scales with the number of steps in exactly the same way $(l_{\min}\sim N^{-2/3})$ as in the case of strong instability $(d_+\gg l)$. Further discussion of this regime will be presented elsewhere.

VIII. UNIVERSALITY CLASSES OF STEP BUNCHING

Before drawing some general conclusions in the next section, here we wish to put our work into the context of a classification scheme for step bunching instabilities proposed by Pimpinelli, Tonchev, Videcoq, and Vladimirova (PTVV).[36] It is based on a generic continuum equation of the form

$$\frac{\partial h}{\partial t}+\frac{\partial}{\partial x}\left[K_1 m^\varrho+\frac{K_2}{m^k}\frac{\partial^2}{\partial x^2}m^n\right]=\text{const}. \qquad (67)$$

Here K_1 and K_2 are material constants with $K_2>0$ and $K_1\varrho>0$, the slope $m=\partial h/\partial x$ is assumed positive everywhere, and ϱ, k, and n are exponents characterizing a class of step bunching instabilities. The exponent n is simply the exponent of the repulsive step interaction, and the exponent k reflects the slope dependence of the surface mobility; $k=1$ and $k=0$ correspond to slow and fast detachment/attachment kinetics, respectively (see Sec. IV). Equation (67) is a slight generalization[39] of the equation proposed in Ref. 36, where only the case $k=0$ was considered.

PTVV argued that the characteristic scaling exponents α and z introduced in Sec. I can be extracted from (67) by requiring that the equation should be invariant under the scale transformation,

$$h(x,t) \Rightarrow b^{-\alpha} h(bx, b^z t), \tag{68}$$

for an arbitrary scale factor b. This yields the expressions

$$\alpha = 1 + \frac{2}{n-k-\varrho}, \quad \gamma = \frac{2}{2+n-k-\varrho},$$
$$z = \frac{2(1+n-k-2\rho)}{n-k-\varrho}, \tag{69}$$

where the scaling relation (3) has been used.

Apart from the symmetry-breaking term in (31), the continuum equation (30) for the sublimation problem is of the generic form (67) with $\varrho=-1$ and $k=1$. It is straightforward to check that, under the rescaling (68), the symmetry-breaking term is smaller by a factor of $b^{-\alpha}$ compared to the leading term $\sim 1/m$, and hence it becomes negligible at large scales; this is consistent with the detailed analysis in Sec. V G. For $\varrho=-1$ and $k=1$ the exponents in (69) reduce to $\alpha=(n+2)/n$ and $\gamma=2/(2+n)$, which we readily recognize as the scaling exponents characteristic of type I solutions [compare to (57)]. To obtain the exponents for type II solutions (which, as was shown in Sec. VII, correctly describe the bunch shape), we must set $\varrho=0$ instead of $\varrho=-1$ in (69).

The reason for the shift in the value of ϱ is evident in view of the considerations of Sec. V C. The scaling argument of PTVV assumes that all terms in (67) are of a similar order of magnitude; in particular, the stabilizing term is balanced against the destabilizing current Bm^{ϱ}. However, for type II solutions the total current is fixed at a value J_0 which is independent of the slope, and which dominates over the term Bm^{ϱ} for large slopes when $\varrho<0$. Thus the stabilizing term is balanced against a slope-independent current, which effectively implies that $\varrho=0$.

The argument clearly extends to any negative value of ϱ, and suggests that generally ϱ should be replaced by $\max(0,\varrho)$. For the continuum evolution equation (63) describing electromigration-induced step bunching in the diffusion-limited regime, which corresponds to $\varrho=1$ and $k=0$, the ambiguity regarding type I and type II solutions does not arise (see Sec. VI A). Since the static exponents α and γ in (69) only depend on the sum $\varrho+k$, it is evident that they take the same values for $\varrho=0$, $k=1$ as for $\varrho=1$, $k=0$; for this reason the static scaling exponents for electromigration-induced step bunching take the same values in the diffusion-limited and the attachment/detachment-limited regimes.

The scaling theory of PTVV also makes predictions about the coarsening behavior of the bunched surface, which our analysis of stationary bunch shapes clearly cannot address. Setting $\varrho=-1$, the expressions (69) yield $\alpha/z=1/2$ for the exponent in the coarsening law (4), which is independent of both n and k; on the other hand, with $\varrho=0$ one obtains $\alpha/z=(n+1)/2n$ for $k=1$. In Fig. 8 we compare numerical data for the temporal evolution of the mean bunch size to these two coarsening laws. The simulations seem consistent with the "superuniversal" value $\alpha/z=1/2$, but also $\alpha/z=3/4$ (for $n=2$) or $2/3$ (for $n=3$) cannot be ruled out. More extensive simulations are needed to firmly pin down the coarsening behavior; this is particularly true here because, in contrast to the static scaling properties discussed earlier in Sec. VII, we do not have any analytic information about the coefficient of the coarsening law. In a recent study of a simple toy model of step bunching, which ignores the repulsive step-step interactions and allows steps to coalesce, it was necessary to go to extremely long times, equivalent to the growth of more than 10^5 monolayers, to ascertain the true asymptotic coarsening behavior.[53]

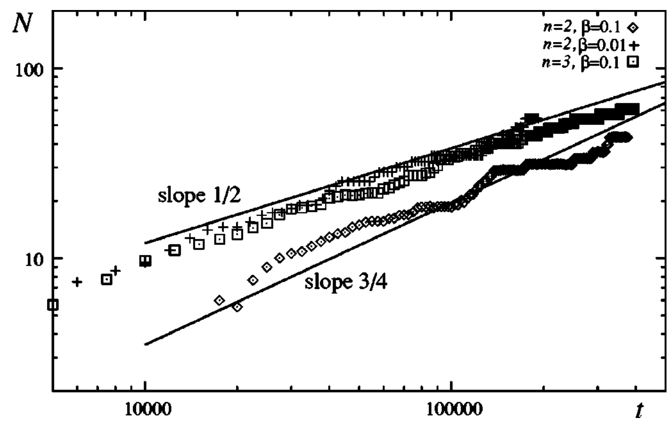

FIG. 8. Time dependence of the mean bunch size for the parameter sets in Figs. 6 and 7, and an additional set with $\beta=0.1$, $\lambda_s/l=100$, $d_+/l=100$, $l_0/l=0.24$, and step interaction exponent $n=3$. The bold lines illustrate the predictions of the scaling theory for $\varrho=-1$ ($\alpha/z=1/2$) and for $\varrho=0$, $n=2$ ($\alpha/z=3/4$).

IX. CONCLUSIONS

In this paper we have presented a detailed analysis of the step bunching instability caused by an Ehrlich-Schwoebel effect during sublimation in the limit of a small desorption rate. When the kinetic length $d_+=D_s/K_+$ is large compared to the average distance between the steps, the instability is strong and bunches of steps appear even at strong repulsion between the steps. In the opposite case (kinetic length d_+ smaller than the interstep distance) the instability is weak and bunches occur only when the step-step repulsion is several orders of magnitude weaker than in the previous case.

A central part of the work is the derivation of the continuum evolution equation in Sec. V, and the careful analysis of its stationary bunch solutions. We have shown that two different types of stationary solutions with different scaling properties can be found, depending on whether the mean surface current J_0 is kept fixed or not. Following Ref. 24, we have argued that J_0 is independent of bunch size, and that the correct bunch shape is given by the type II solution, which describes a bunch of finite extent with Pokrovsky-Talapov-type singularities at the edges. This is confirmed by the excellent agreement with numerical simulation results for the minimal interstep spacing $l_{\min}$ and the first interstep spacing in the bunch l_1 presented in Sec. VII.

On the other hand, we find noticeable deviations of the behavior of the total bunch width L from the type II prediction. We suggest that the discrepancy may be related to the distinct asymmetry between the leading and the trailing edges of the bunch: The terraces between the crossing steps escaping from the leading edge of the bunch appear to contribute strongly to the total bunch width, to the extent that asymptotically L may be considerably larger than $Nl_{\min}$. Further clarification of the issue requires a better understanding of the motion of bunches and the interactions between bunches, which is beyond the scope of the present paper.

Our work has important consequences for the recently proposed scenario of universality classes for step bunching instabilities.[36] First, we have pointed out the mathematical equivalence between appropriate limits of the step bunching instabilities caused by sublimation, growth and electromigration on the levels of *both* discrete step dynamics and continuum evolution equations. This equivalence gives a very clear meaning to the notion of a universality class, and we believe that the particular class considered in this paper (characterized, in essence, by the linearity of the destabilizing terms in the step equations) is in fact relevant to a wide range of experimentally realized systems. As a practical matter, the unified view provided by the continuum approach allows us to derive explicit formulas for the bunch shape which, through the identification of the scaling parameter S, are directly applicable to these diverse realizations of step bunching. Second, we have shown that the procedure employed in Ref. 36 to extract the scaling exponents from the continuum evolution equation captures only one type of solution (the type I solutions of Sec. V C), which is not the relevant one at least as far as the time-independent scaling properties are concerned.

A crucial question that should be addressed in future work concerns the coarsening behavior of the bunched surface, and the relationship between coarsening dynamics and bunch motion. As was discussed in Sec. VIII, the present work remains inconclusive on this point. It is remarkable, however, that a very robust scaling of the mean bunch size and bunch spacing as $N \sim \xi \sim t^{1/2}$ has been observed in a number of numerical simulations, both for electromigration[20,24,26] and growth with inverse ES barriers,[12,14] as well as in an experimental study of electromigration-induced step bunching on Si(111).[19] Liu and Weeks[24] have proposed an elegant explanation for the ubiquity of the $t^{1/2}$ scaling within a continuum setting; their argument presupposes, however, as does the scaling approach of PTVV,[36] that the bunch spacing ξ is the only lateral length scale in the problem, although the bunch width L clearly comes into play as well.[39] This remains true even if the internal bunch structure is eliminated by allowing the steps to coalesce.[53] Thus the origin of the observed temporal scaling remains to be understood.

ACKNOWLEDGMENTS

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[1] P. Venezuela, J. Tersoff, J. A. Floro, E. Chason, D. M. Follstaedt, Feng Liu, and M. G. Lagally, Nature (London) **397**, 678 (1999).
[2] C. Teichert, Phys. Rep. **365**, 335 (2002).
[3] N. Néel, T. Maroutian, L. Douillard, and H.-J. Ernst, J. Phys.: Condens. Matter **15**, S3227 (2003).
[4] M. Syväjärvi, R. Yakimova, and E. Janzén, J. Cryst. Growth **236**, 297 (2002).
[5] O. Gliko, N. Booth, and P. G. Vekilov, Acta Crystallogr., Sect. D: Biol. Crystallogr. **D58**, 1622 (2002).
[6] O. Gliko, I. Reviakine, and P. G. Vekilov, Phys. Rev. Lett. **90**, 225503 (2003).
[7] J. Tersoff, Y. H. Phang, Z. Zhang, and M. G. Lagally, Phys. Rev. Lett. **75**, 2730 (1995).
[8] F. Liu, J. Tersoff, and M. G. Lagally, Phys. Rev. Lett. **80**, 1268 (1998).
[9] R. L. Schwoebel, J. Appl. Phys. **40**, 614 (1969).
[10] A. Pimpinelli, I. Elkinani, A. Karma, C. Misbah, and J. Villain, J. Phys.: Condens. Matter **6**, 2661 (1994).
[11] M. Uwaha, Y. Saito, and M. Sato, J. Cryst. Growth **146**, 164 (1995).
[12] M. Sato and M. Uwaha, Surf. Sci. **493**, 494 (2001).
[13] M. H. Xie, S. Y. Leung, and S. Y. Tong, Surf. Sci. **515**, L459 (2002).
[14] V. Tonchev, J. Krug, H. Omi, Y. Homma, and A. Pimpinelli (unpublished).
[15] A. V. Latyshev, A. L. Aseev, A. B. Krasilnikov, and S. I. Stenin, Surf. Sci. **213**, 157 (1989).
[16] Y. Homma, R. J. Mcclelland, and H. Hibino, Jpn. J. Appl. Phys., Part 2 **29**, L2254 (1990).
[17] S. Stoyanov, Jpn. J. Appl. Phys., Part 1 **30**, 1 (1991).
[18] B. Houchmandzadeh, C. Misbah, and A. Pimpinelli, J. Phys. I **4**, 1843 (1994).
[19] Y.-N. Yang, E. S. Fu, and E. D. Williams, Surf. Sci. **356**, 101 (1996).
[20] H. Dobbs and J. Krug, J. Phys. I **6**, 413 (1996).
[21] S. Stoyanov, in *Surface Diffusion—Atomistic and Collective Processes*, edited by M. Tringides (Plenum, New York, 1997), p. 285.
[22] S. Stoyanov, Surf. Sci. **370**, 345 (1997).
[23] E. S. Fu, D.-J. Liu, M. D. Johnson, J. D. Weeks, and E. D. Williams, Surf. Sci. **385**, 259 (1997).
[24] D.-J. Liu and J. D. Weeks, Phys. Rev. B **57**, 14891 (1998).
[25] J. J. Métois and S. Stoyanov, Surf. Sci. **440**, 407 (1999).
[26] M. Sato and M. Uwaha, Surf. Sci. **442**, 318 (1999).

[27] K. Yagi, H. Minoda, and M. Degawa, Surf. Sci. Rep. **43**, 45 (2001).
[28] H. Minoda, J. Phys.: Condens. Matter **15**, S3255 (2003).
[29] S. Stoyanov and V. Tonchev, Phys. Rev. B **58**, 1590 (1998).
[30] S. Stoyanov, Surf. Sci. **416**, 200 (1998).
[31] K. Fujita, M. Ichikawa, and S. S. Stoyanov, Phys. Rev. B **60**, 16006 (1999).
[32] Y. Homma and N. Aizawa, Phys. Rev. B **62**, 8323 (2000).
[33] S. Stoyanov, J. J. Métois, and V. Tonchev, Surf. Sci. **465**, 227 (2000).
[34] S. Stoyanov, Surf. Sci. **464**, L715 (2000).
[35] P. Nozières, in *Solids Far From Equilibrium*, edited by C. Godrèche (Cambridge University Press, Cambridge, 1991).
[36] A. Pimpinelli, V. Tonchev, A. Videcoq, and M. Vladimirova, Phys. Rev. Lett. **88**, 206103 (2002).
[37] W. Burton, N. Carbrera, and F. C. Frank, Philos. Trans. R. Soc. London, Ser. A **243**, 299 (1951).
[38] J. Krug, in *Multiscale Modeling of Epitaxial Growth*, edited by A. Voigt (Birkhäuser, 2005).
[39] J. Krug, in *Collective Dynamics of Nonlinear and Disordered Systems*, edited by G. Radons, P. Häussler, and W. Just (Springer, Berlin, 2005). p. 5.
[40] T. Michely and J. Krug, *Islands, Mounds and Atoms. Patterns and Processes in Crystal Growth Far from Equilibrium* (Springer, Berlin, 2004).
[41] W. F. Chung and M. S. Altman, Phys. Rev. B **66**, 075338 (2002).
[42] J. Krug, in *Dynamics of Fluctuating Interfaces and Related Phenomena*, edited by D. Kim *et al.* (World Scientific, Singapore, 1997), p. 95.
[43] F. C. Frank, in *Growth and Perfection of Crystals*, edited by R. Doremus, B. Roberts, and D. Turnbull (Wiley, New York, 1962), p. 411.
[44] P. Nozières, J. Phys. (Paris) **48**, 1605 (1987).
[45] D.-J. Liu, E. S. Fu, M. D. Johnson, J. D. Weeks, and E. D. Williams, J. Vac. Sci. Technol. B **14**, 2799 (1996).
[46] F. Lançon and J. Villain, in *Kinetics of Ordering and Growth at Surfaces*, edited by M. Lagally (Plenum, New York, 1990).
[47] W. W. Mullins, J. Appl. Phys. **30**, 77 (1959).
[48] P. Politi and J. Villain, Phys. Rev. B **54**, 5114 (1996).
[49] J. Villain, J. Phys. I **1**, 19 (1991).
[50] J. Krug, M. Plischke, and M. Siegert, Phys. Rev. Lett. **70**, 3271 (1993).
[51] P. Politi, G. Grenet, A. Marty, A. Ponchet, and J. Villain, Phys. Rep. **324**, 271 (2000).
[52] J. Myslivеček, C. Schelling, F. Schäffler, G. Springholz, P. Šmilauer, J. Krug, and B. Voigtländer, Surf. Sci. **520**, 193 (2002).
[53] F. Slanina, J. Krug, and M. Kotrla, cond-mat/0409324 (unpublished).