Shape and scaling of moving step bunches

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Abstract. – We study step bunching under conditions of attachment/detachment limited kinetics in the presence of a deposition or sublimation flux, which leads to bunch motion. Analysis of the discrete step dynamics reveals that the bunch velocity is inversely proportional to the bunch size for general step-step interactions. The shape of steadily moving bunches is studied within a continuum theory, and analytic expressions for the bunch profile are derived. Scaling laws obtained previously for non-moving bunches are recovered asymptotically, but singularities of the static theory are removed and strong corrections to scaling are found. The size of the largest terrace between two bunches is identified as a central scaling parameter. Our theory applies to a large class of bunching instabilities, including sublimation with attachment asymmetry and surface electromigration in the presence of sublimation or growth.

Introduction. – There is much current interest in exploiting morphological instabilities to form periodic nanoscale patterns at crystal surfaces [1, 2]. Because of their natural in-plane anisotropy, vicinal surfaces [3] prepared at a miscut relative to a high symmetry orientation provide ideal substrates for the formation of ripple patterns parallel or perpendicular to the mean step orientation [4, 5]. Here we specifically consider patterns formed by step bunching, the process in which a train of initially equally spaced (straight) steps splits into regions of densely packed steps (step bunches), and almost flat regions [6, 7]. Bunched semiconductor surfaces are promising templates for the growth of metallic nanowires [8].

Step bunching can be induced by growth [9, 10], sublimation [11], or surface migration of adatoms driven by an electric current [4, 12–18]. The common feature of the different instability mechanisms [7] is that they break the symmetry between the ascending and descending steps bordering a terrace. The appearance of step bunches thus provides information about the asymmetry of the attachment/detachment processes at the steps, as well as about the direction of current-induced adatom migration. Once formed, the shape of a bunch is determined by the balance between the destabilizing forces and the repulsive step-step interactions that act to regularize the step train. As a result, the bunch shape displays characteristic scaling laws relating e.g. its slope and width to the number of steps in the bunch [13, 14]. These scaling laws are used in the interpretation of experiments to extract the functional form
of the step interactions as well as material parameters such as the step interaction strength and the electromigration force [17, 18].

The large scale properties of step bunches are captured by continuum evolution equations for the surface profile [6], which can be derived from the underlying discrete step dynamics in a systematic manner [11]. The analysis of static (time-independent) solutions of these equations leads to scaling laws which are in reasonable agreement with numerical simulation of the discrete step dynamics [11]. However, in the presence of a non-vanishing sublimation or growth flux, step bunches are moving objects. Because of the high temperatures involved, sublimation — and hence, bunch motion — is significant also in electromigration experiments, where it is not the primary cause of bunching [12, 15].

In this Letter we show that bunch motion alters the shape and scaling properties of bunches in a fundamental way. It removes the artificial symmetry between the in-flow and out-flow regions (in which steps move into and out of the bunch, respectively) and the concomitant singularities of the static solutions at the bunch edges [11]. We show that the lateral speed of a bunch is inversely proportional to its height for a large class of models, and we identify the size of the largest terrace $l_{\text{max}}$ as a natural scaling parameter, in terms of which other important bunch characteristics are expressed in a simple way. The maximal terrace size $l_{\text{max}}$ is uniquely defined, in contrast to the number of steps in the bunch, which requires a convention to decide which steps belong to it, and it is directly accessible experimentally by means of reflection electron microscopy (REM) [16].

Discrete model. — We consider a system of non-transparent steps [7] described on the discrete level by the equations of motion

$$\frac{dx_i}{dt} = \frac{1 - b}{2} (x_{i+1} - x_i) + \frac{1 + b}{2} (x_i - x_{i-1}) + U (2f_i - f_{i-1} - f_{i+1})$$

(1)

for the step positions $x_i(t)$, where the time scale has been normalized to the growth or sublimation flux. The parameter $b$ governs the asymmetry between ascending and descending steps, relative to the mean step velocity. The linear form of the first two terms on the right hand side of (1) is characteristic of slow attachment/detachment kinetics, and applies equally to step bunching induced by sublimation, growth or surface electromigration [11, 14]; here we will assume a sublimating step train going uphill in the $+x$ direction. The last term on the right hand side of (1) represents stabilizing step-step interactions of strength $U$. In the usual case of entropic or dipolar elastic interactions

$$f_i = \left( \frac{l}{x_{i} - x_{i-1}} \right)^{\nu+1} - \left( \frac{l}{x_{i+1} - x_{i}} \right)^{\nu+1},$$

(2)

where $\nu = 2$ and $l$ is the average terrace length [3]. Explicit expressions for $b$ and $U$ in terms of physical parameters are given below in (15).

For $b > 0$, (1) leads to an instability of the equally spaced step configuration $x_i - x_{i-1} = l$ and its segregation into step bunches separated by flat regions. The bunches coarsen slowly in time by coalescence. We are interested in the final regime of coarsening with a few big bunches left in the system. In this regime, one can study a periodic array of identical bunches, each containing $M$ steps, which satisfy (1) with $i = 1, 2, ..., M$ and the helicoidal boundary conditions $x_{M+1} = x_1 + Ml$. It is convenient to consider the comoving step coordinates $y_i(t) = x_i(t) - lt$, in which the center of mass of the step configuration does not move. In this frame, the stationary trajectory of a step is a periodic function with some (unknown) period $\tau$, $y_i(t) = y_i(t + \tau)$. Stationarity implies that every step follows the same trajectory, up to a space and time shift,
according to \( y_{i+s}(t) = y_i(t + \tau s/M) + ls \), with \( s = 1, 2, \ldots, M - 1 \). Inserting this into (11) and setting \( \Delta(t) = y_{i+1}(t) - y_i(t) \) we obtain an equation for the stationary step trajectory (in the following we omit subscripts)

\[
\frac{dy}{dt} = \frac{1-b}{2} \Delta(t) + \frac{1+b}{2} \Delta(t - \frac{\tau}{M}) - l + U \left[ 2f(t) - f(t - \frac{\tau}{M}) - f(t + \frac{\tau}{M}) \right].
\]

(3)

This is a differential-difference equation for two periodic functions \( y(t) \) and \( f(t) \), which for the time being will be treated as independent. Expanding the functions in Fourier series with frequencies \( w_n = 2\pi n/\tau \) and coefficients \( Y_n \) and \( F_n \), respectively, we obtain from (3)

\[
w_n = \sin \frac{2\pi n}{M} + 2U \left( 1 - \cos \frac{2\pi n}{M} \right) \text{Im}[F_n/Y_n].
\]

(4)

Since (11) is valid for any \( n \), we can choose \( n/M \ll 1 \) for large \( M \) and expand (4) to obtain the expression \( \tau = M - 2\pi U \text{Im}[nF_n/Y_n] + O(M^{-1}) \), which in fact determines the dependence of the bunch velocity on \( M \). In the laboratory frame we have \( x_i(t + \tau/M) = x_{i+1}(t) + l(\tau/M - 1) \), which implies that the whole step configuration shifts by \( l(\tau/M - 1) \) to the right in time \( \tau/M \). Hence the lateral bunch speed \( v \) is given by

\[
v/l = 1 - M/\tau = \kappa/M + o(M^{-1}),
\]

(5)

where \( \kappa = -2\pi U \text{Im}[nF_n/Y_n] \) has to be determined self-consistently for a given form of step-step interaction. When \( f \) has the usual form (2) with \( \nu = 2 \), we find numerically that \( \kappa \) is a constant proportional to the asymmetry, \( \kappa \approx 3b \), provided that the asymmetry is not too large, \( b \leq 0.5 \).

In the following we will see that even though the bunch velocity decreases with increasing bunch size, it cannot be neglected. According to a scaling argument due to Chernov [9,13,19], the scaling \( v \sim M^{-1} \) implies that the average bunch size should increase with time as \( \sqrt{t} \), which is consistent with experiments [12,18] and numerous discrete simulation [14,15].

**Continuum theory.** – The continuum evolution equation corresponding to the discrete dynamics (11) reads [11]

\[
\frac{\partial h}{\partial t} + \frac{\partial}{\partial x} \left[ \frac{bh^2}{2m} - \frac{h^3}{6m^2} \frac{\partial m}{\partial x} + \frac{3U^3}{2m} \frac{\partial^2 (m^2)}{\partial x^2} \right] + h_0 = 0,
\]

(6)

where \( h(x,t) \) is the surface profile, \( m(x,t) = \partial h/\partial x > 0 \) is the slope, and \( h_0 \) denotes the height of a single step. A periodic array of bunches moving at lateral speed \( v \) is obtained by the travelling wave ansatz [9] \( h(x,t) = h(\xi) + \Omega t - h_0 \), where \( \xi = x - vt \) and the function \( h(\xi) \) satisfies the boundary condition \( h(\xi + Ml) = h(\xi) + Mh_0 \). Inserting this into (6) we find that the vertical excess speed \( \Omega \) is related to \( v \) by \( \Omega = vm_0 \), where \( m_0 = h_0/l \) is the average slope. Integrating once the ordinary differential equation for \( h(\xi) \) then becomes

\[
\Omega (\xi + \xi_0 - h) + \frac{b}{2} \left( 1 - \frac{1}{m} \right) - \frac{m'}{6m^3} + \frac{3U}{2m} (m^2)'' = 0.
\]

(7)

We denote derivatives by primes, and measure lateral distances in units of \( l \) and heights in units of \( h_0 \). The phase shift \( \xi_0 \) is a constant of integration satisfying the condition \[\int_0^M m(\xi) (h(\xi) - \xi - \xi_0) d\xi = 0\], which follows by multiplying (7) by \( m \), integrating over the bunch period, and using the boundary conditions. For future reference we note that, for small \( b, \ \Omega \approx 3b/M \) because of (5).
Fig. 1 – Shape of a moving bunch $h(\xi)$ computed from the discrete dynamics $\bullet$ [symbols], and the continuous evolution equation $\bullet$ [full line], for 128 steps with $b = 3/17 \approx 0.17647$, and $U = 0.569$. There are no fitting parameters.

Fig. 2 – Slope profile derived from Fig.1 for a moving bunch (full curve) and a static bunch (bold dashed curve). The slope of the moving bunch increases abruptly in the inflow region and decreases gradually in the outflow region.

In Fig.1 a numerical solution of (7) obtained via a shooting method is compared to the discrete step dynamics, showing excellent agreement. The continuum description is generally found to work very well, provided the asymmetry $b$ is sufficiently small. In Fig.2 we compare the corresponding slope profile to the time-independent solution derived in [11] by setting the terms inside the square brackets in (6) to zero and neglecting the symmetry-breaking term $(h_0^3/6m^3)\partial m/\partial x$. As was anticipated in [11], the moving bunch is distinctly asymmetric. Moreover the moving solution extends smoothly over the whole $x$-axis, whereas the static solution has finite support due to singularities at the bunch edges. In the following we find analytically the asymptotics of the inflow and outflow regions of the moving bunch, corresponding to the extreme left and right parts of Fig.1 (see also Fig.2).

Outflow region: $m(\xi) \ll 1$, $m'(\xi) < 0$. – In this region the steps are far apart and their interaction $U$ is negligible. It is convenient to perform a Lagrange transform from the function $h(\xi)$ to its inverse $\xi = \xi(h)$. After some algebra $\bullet$ with $U = 0$ then reduces to the linear equation

$$\xi'' - 3b\xi' + 6\Omega\xi = 6\Omega(h - \xi_0) - 3b,$$

which has the general solution

$$\xi = h - \xi_0 + C_1 \exp(\lambda_1 h) + C_2 \exp(\lambda_2 h)$$

with $\lambda_{1,2} = (3b/2)[1 \pm \sqrt{1 - 8\Omega/3b^2}]$. Fixing the boundary conditions so that the point of minimal slope $\min_\xi m(\xi) = \varepsilon$ is located at $h = 0$, we have two boundary conditions $\xi(0) = 0$ and $\xi'(0) = 1/\varepsilon$ to determine $C_1, C_2$. Recalling that $\Omega \approx 3b/M$, we see that $\lambda_1 \to 3b$ and $\lambda_2 \to 0$ for large bunches, so that (10) becomes a pure exponential, corresponding to a slope profile $m(\xi) \approx 1/(3b\xi)$. Similar behavior was found in a model with short-range step interaction, however in that case $\Omega \to 3b^2/8$ and $\lambda_1 \to \lambda_2$ for large bunches [9].

Inflow region: $m(\xi) \ll m_{\max}$, $m'(\xi) \geq 0$. – In this region one can neglect the first two terms in (10), as can be shown by a careful analysis of (12). The remaining terms give
\[ 9U(m^2)'' = m'/m^2. \] Integrating once, we find \( 9U(m^2)' = -m^{-1} + \varepsilon^{-1} \) by requiring the derivative \( m'(\xi) \) to vanish at the point with minimal slope \( \varepsilon \). Integrating again, we obtain an implicit equation for \( m(\xi) \),

\[ 18U\varepsilon \left[ m^2/2 + m\varepsilon + \varepsilon^2 \ln(m/\varepsilon - 1) \right] = \xi. \] (10)

Note that (10) is valid for \( m(\xi) > \varepsilon + 0 \), to avoid the logarithmic singularity at \( m = \varepsilon \). In reality there is no singularity, because additional terms from (7) have to be included when \( m \to \varepsilon \), which however are completely irrelevant in the remaining part of the inflow region.

**Scaling laws.** – We are now prepared to investigate the scaling properties of large step bunches (\( M \gg 1 \)).

(A) The easiest is to find the size of the first terrace in the bunch \( l_1 \), defined as in [11] by \( m(h = h_0) = h_0/l_1 \), since this region is well described by (10). Away from the singularity, for \( m \gg \varepsilon \), (10) reduces to \( m(\xi) \approx \sqrt{\varepsilon/9U\varepsilon} \), which is of a similar form as the Pokrovsky-Talapov singularity found for static bunches [11]. This yields immediately

\[ l_1 \approx (6U\varepsilon)^{1/3}. \] (11)

(B) To estimate the size of the minimal terrace in the bunch \( l_{\min} = 1/m_{\max} \), we multiply (7) by \( m(m^2)' = 2m^2m' = (2/3)(m^3)' \) and integrate from \( \xi_1 \) to \( \xi_2 \):

\[ \left[ \frac{3U}{4} \left( (m^2)' \right)^2 + b \left( \frac{m^3}{3} - \frac{m^2}{2} \right) \right] \xi_2 \approx -2\Omega \int_{\xi_1}^{\xi_2} m^2m' (\xi + \xi_0 - h) d\xi + \frac{1}{3} \int_{\xi_1}^{\xi_2} \frac{(m')^2}{m} d\xi. \] (12)

Setting \( \xi_1 = 0 \), \( m(0) = \varepsilon \) and \( \xi_2 = \xi_{\max} \) with \( m(\xi_{\max}) = m_{\max} \), the left hand side gives \( \approx bm^3_{\max}/3 \) for \( m_{\max} \gg 1 \). The second integral on the right hand side can be taken, noting that the function \( (m')^2/m \) vanishes everywhere except in the narrow inflow region, where (10) holds, yielding \( \int_{\xi_1}^{\xi_{\max}} (m')^2/m d\xi = \left[-m' - (36U/m^2)^{-1}\right]_{\xi_1}^{\xi_{\max}} \approx (36U\varepsilon)^{-1} \equiv I_0 \). To estimate the first integral, first set \( \xi_2 = M \) in (12) so that the left hand side vanishes due to the periodic boundary conditions. We obtain then \( I_0 [0, M] = 2\Omega \int_0^M m^2m' (\xi + \xi_0 - h) d\xi \approx I_0/3 \). Denoting by \( \gamma = \lim_{M \rightarrow \infty} I_1 [0, \xi_{\max}] / I_1 [0, M] \) the relative contribution to the integral from the segment \([0, \xi_{\max}]\) for large \( M \), we find from (12) \( bm^3_{\max} \approx (1 - \gamma) I_0 \), or

\[ m_{\max}^{-1} = l_{\min} \approx \left( \frac{36U\varepsilon^2b}{1 - \gamma} \right)^{1/3}. \] (13)

Numerically we observe that the value of \( \gamma \) indeed saturates to a fixed value for large \( M \), and depends rather weakly on \( b \) and \( U \). Varying \( b \) and \( U \) around physically relevant choices of parameters, e.g., those in Fig.1 or in [11], we find \( \gamma \approx 0.7 \pm 0.01 \).

(C) **Bunch width.** The definition of the bunch width depends on the convention used to assign steps to the bunch [11]. Here we define the bunch as the collection of terraces with sizes smaller than the mean terrace size \( l \). We can obtain an estimate of \( W \) integrating the first term on the right hand side of (12) by parts: \( \int_0^M m^2m' (\xi + \xi_0 - h) d\xi = (1/3) \int_0^M m^3 (m - 1) d\xi \), and arguing that the dominant contribution to the integral comes from the bunch interior. Then \( \int_0^M m^3 (m - 1) d\xi \approx \int_0^W m^3 d\xi = Qm^3_{\max} W = MI_0/(6b) \), where \( Q < 1 \), and we have used \( \Omega \approx 3b/M \). Substituting \( m_{\max} \) we get

\[ W = \frac{Q^{-1}M}{6(1 - \gamma)^{4/3}} \left( 36U\varepsilon^2b \right)^{1/3}. \] (14)
For the parameters of Fig.1 $Q \approx 0.3237$ for large $M$, and it changes only slightly ($\pm 2\%$) under significant variations of $b$ and $U$.

(D) The minimal slope. As we have seen, many characteristics of the moving bunch are controlled by the single parameter $\varepsilon$, which can be defined microscopically as the inverse size of the largest terrace in the outflow region between two consecutive bunches, $l_{\text{max}} = 1/\varepsilon$. In order to make a connection to earlier studies, we need the dependence of $\varepsilon$ on the bunch size $M$. From the asymptotic slope profile $m \approx 1/(3b\xi)$ in the outflow region, one expects $\varepsilon \approx (3bM)^{-1}$ to leading order. Numerical studies suggest however strong finite size corrections even for large bunches, $M \lesssim 200$. The behaviour of $\varepsilon$ is rather well approximated by $\varepsilon^{-1} \approx 3b\alpha M - A(b,U)$ where $\alpha \lesssim 1$ and typically $A$ is not small, e.g., for $b,U$ from Fig.1 $A \approx 13$ in the range of bunch sizes $50 \leq M \leq 550$.

If we nevertheless use the asymptotic expression $\varepsilon \approx (3bM)^{-1}$ in (11)-(14) we recover the scaling laws derived in [11] for static bunches, however with different numerical prefactors. This provides an a posteriori justification for the agreement between the predictions for static bunches and the numerical data in [11]. Noting that the dimensionless parameter $S$ introduced in [11] is given by $S = U/(b(\ell_{\text{min}}))$ in the present units, we see that (11) and (13) reduce to $l_1 \approx (2S/M)^{1/3}$ and $l_{\text{min}} \approx (13.3 \times S/M^2)^{1/3}$, which is to be compared with the expressions $l_1 = (4S/M)^{1/3}$ and $l_{\text{min}} = (16S/M^2)^{1/3}$ for static bunches. From (14) we find that the ratio $W/(Ml_{\text{min}}) = [6Q(1-\gamma)]^{-1} \approx 1.72$, which is considerably larger than the corresponding number 1.29 in the static case. This reflects the fact that moving bunches are considerably broader than their static counterparts, because of the gradual increase of the terrace sizes in the outflow region, and explains the significant discrepancy between numerical and analytic estimates for $W$ in [11]. Finally, we note that for a general step-step interaction exponent $\nu$ in (2) we arrive at generalized scaling laws $l_1 \sim \varepsilon^{1/(\nu+1)}$, $l_{\text{min}} \sim \varepsilon^{2/(\nu+1)}$ and $W \sim \varepsilon^{-1/(\nu+1)}$ which are, apart from strong finite size corrections, consistent with the ones derived in [11].

Experimental considerations. – An important condition for the applicability of our continuum theory is the smallness of the asymmetry parameter, $b \leq 0.5$. For step bunching induced by a conventional Ehrlich-Schwoebel (ES) effect during sublimation, $b = (k_+ - k_-)/(k_+ + k_-)$, where $k_+$ ($k_-$) is the kinetic coefficient for attachment to a step from the lower (upper) terrace [11]; keeping $b$ small then simply requires a weak ES effect. For current-induced step bunching in the attachment/detachment limited regime, one finds [14]

$$b = \frac{k c_{eq} a^2 F \tau_e}{k_B T} = \frac{\Gamma F \tau_e}{2 a^2 k_B T}, \quad U = \frac{\Gamma g \tau_e m_0^3}{2 k_B T}$$

where $k = k_+ = k_-$ denotes the attachment rate of adatoms to steps, $a^2$ the atomic area, $c_{eq}$ the equilibrium adatom concentration, $F$ the electromigration force, $\tau_e$ the monolayer evaporation time, and $g$ the step interaction strength. The quantity $\Gamma = 2 k c_{eq} a^4$ is the mobility of an isolated step. The model (1) of non-transparent steps is expected to apply in two of the four temperature regimes [4] in which step bunching is observed on Si(111), around 900$^\circ$ C and around 1250$^\circ$ C [16–18]. The material parameters given in [12,14] lead to the estimate $b \approx 14$ in the low temperature regime and $b \approx 0.3$ in the high temperature regime. The latter is presumably an upper bound, since a recent estimate [20] of the kinetic length [7] $l_k = D/k$ (where $D$ is the adatom diffusion coefficient) at 1200$^\circ$ C indicates that the step mobility $\Gamma$ increases less rapidly with increasing temperature than was assumed in [12]. The step interaction parameter $U$ depends very sensitively on the mean miscut $m_0 = h_0 / l$. Taking the interaction strength to be $g \approx 0.1$ eV/Å$^2$ at 1250$^\circ$ C, the parameters given in [12,14] yield $U/l \approx 0.2$ for $l = 50$ nm.
Conclusions. – In this paper we have shown that the continuum equation (6) faithfully represents the properties of moving step bunches for sufficiently small values of $b$, and that it can be used to extract accurate analytic expressions for the bunch shape and its various characteristic length scales. Our study reveals a central role of the point of minimal slope (or maximal terrace size) where the outflow region of one bunch joins the inflow region of the next. An important ingredient is a Fourier analysis of the discrete equations of step motion, which yields an inverse dependence of the bunch speed on bunch size under rather general conditions. Further work is needed to analytically derive the coefficient $\kappa$ in (5), and to understand how to obtain the bunch speed directly from the continuum equation, possibly by exploiting a recently proposed analogy to front propagation problems [9]. In addition, it seems desirable to study the regime of large $b$, and to investigate the consequences of bunch motion for bunch coarsening beyond simple scaling arguments [9, 19].

The conditions assumed in this paper should be realizable in electromigration experiments on Si(111) at temperatures around 1250°C. The gross features of the morphology, such as the maximal terrace size $l_{\text{max}}$ and the bunch width $W$, could be followed in real time using REM, while for the more delicate measurements of $l_{\text{min}}$ and $l_{1}$ STM-studies would be preferable.

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