Introduction to Step Dynamics and Step Instabilities

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Abstract. This paper provides an elementary introduction to the basic concepts used in describing epitaxial crystal growth in terms of the thermodynamics and kinetics of atomic steps. Selected applications to morphological instabilities of stepped surfaces are reviewed, and some open problems are outlined.

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1. Introduction

The hallmark of a crystalline solid is the discrete translational symmetry imposed by the crystal lattice. At the surface of a crystal, this leads to the existence of atomic steps, which separate exposed lattice planes (terraces) that differ in height by a single lattice spacing. At sufficiently low temperatures, steps are thermodynamically stable, in the sense that the creation of a new step segment entails a positive free energy cost per unit length of the step. Thus steps are long-lived surface defects, which makes them suitable as a basis for the description of the surface morphology on an intermediate (mesoscopic) scale, between atomistic and macroscopic levels of modeling.

In crystal growth, steps play a central role because they provide the kink sites at which new atomic units are incorporated into the crystal (see Fig.1). The growth of a crystal surface can thus be reduced to the advancement of existing steps, the nucleation of new closed step loops (i.e., atomic height islands), and the annihilation of steps by the merging of islands and terraces. This point of view was pioneered by Burton, Cabrera and Frank (BCF) in their classic 1951 paper [1]. The exchange of matter between the steps and the population of adsorbed atoms

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(adatoms) on the terraces implies that the step motion has to be formulated as a moving boundary problem. With the advent of powerful numerical techniques for the solution of such problems, step dynamics has become an attractive alternative to atomistic modeling approaches in epitaxial crystal growth. Recent progress along these lines is described in many contributions to this volume.

The main purpose of the present article is to introduce the basic concepts used in the step-dynamical approach to crystal growth. Since this approach is most useful when the number of steps is conserved, i.e. in the absence of island nucleation and merging, we will largely restrict ourselves to the growth on stepped (vicinal) surfaces. In Sects. 2 and 3 we will present the fundamental thermodynamic and kinetic notions in a reasonably self-contained manner, with considerable attention to physical assumptions and approximations that enter into the construction of the model. Sections 4 and 5 provide a brief overview of applications to morphological instabilities of stepped surfaces. Here the discussion will be rather cursory, but key references will be given to guide the reader into the extensive literature. In the final section we try to formulate some challenges for the future. General introductions to the subject can be found, e.g., in [2,3,4].

2. Thermodynamics of steps

The fundamental abstraction of the step-dynamical approach is the replacement of the microscopic step conformation, which is a (possibly very convoluted) path on the discrete surface lattice, by a smooth curve in continuous space. At least locally, the step can then be described by the graph of a function $y(x)$ (Fig. 1).

2.1. Step free energy and step stiffness

The thermodynamic properties of a single step are contained in the step free energy per unit length $\delta$ which, because of the underlying crystal structure, is generally a function $\delta(\theta)$ of the in-plane step orientation angle $\theta$ (see Fig. 1). The step is a long-lived, thermodynamically stable object as long as $\delta > 0$. At the thermal roughening transition of the surface the step free energy vanishes. Above the roughening transition temperature $T_R$ steps proliferate and a description of the surface in terms of isolated steps and flat terraces is no longer possible. The concept of a roughening transition was first conceived by BCF [1], but the nature of the transition was clarified only much later, in the seventies of the past century [5,6]. For applications to epitaxial growth the roughening transition is of little importance, as the growth processes of interest usually proceed far below $T_R$.

Given the function $\delta(\theta)$, the free energy $F$ of an arbitrary step configuration $y(x)$ is obtained by integrating along the step,

$$F = \int ds \, \delta(\theta(s)) = \int dx \, \sqrt{1 + (dy/dx)^2} \, \delta(\theta(x)),$$

where $s$ denotes the arc length along the step and $\theta(x) = \arctan(dy/dx)$. From [2.1] the step chemical potential, i.e., the free energy change upon adding an atom
to the step, can be derived by functional differentiation. This yields the expression

$$\mu = \Omega \frac{\delta F}{\delta y} = \Omega \tilde{\delta} \kappa,$$

(2.2)

where $\Omega$ denotes the area occupied by a surface atom, $\kappa$ is the step curvature, and the quantity $\tilde{\delta} = \delta + d^2 \delta/d\theta^2$ is known as the stiffness of the step. The step stiffness appears in a local version of the Wulff construction, which relates the step free energy to the equilibrium shape of two-dimensional islands [4, 6]. In this formulation the equilibrium condition reads simply

$$\tilde{\delta} \kappa = \text{const.},$$

(2.3)

i.e. the local curvature of the equilibrium shape is inversely proportional to the local step stiffness.

The calculation of $\delta(\theta)$ for a specific system requires the application of equilibrium statistical mechanics to a microscopic model of the surface. A popular microscopic model is the Ising lattice gas, where each site of the surface lattice is
either vacant or occupied and the energy of a configuration is obtained by sum-
mixing over all pairs of occupied nearest neighbor sites. A simple, model-independent
expression for the step stiffness is obtained for steps along the close-packed (=
minimal energy) directions of the lattice at low temperatures. Such steps consist
of straight close-packed segments interspersed by a small concentration of kinks.
Elementary statistical mechanics considerations then show that

$$\tilde{\delta} \approx \frac{k_B T}{2a} e^{\epsilon T / k_B T},$$

(2.4)

where $k_B$ denotes Boltzmann’s constant, $T$ is the temperature, $a$ the in-plane
lattice spacing, and $\epsilon$ is the energy cost of a kink.

2.2. Step roughness

The existence of a roughening transition for two-dimensional surfaces, which was
briefly mentioned in the preceding subsection, is due to the fact that steps are
extended, one-dimensional objects. As a consequence the free energy of a step
increases with its length (provided $\delta > 0$), and the free energy cost for the sponta-
aneous creation of a macroscopic piece of a step becomes prohibitively large. In
contrast, the creation of a kink on a one-dimensional step requires only a fixed en-
ergy amount $\epsilon$, and hence a step contains a finite kink concentration at any non-
zero temperature. This implies that the step is rough whenever $T > 0$: A typical step
conformation looks like the graph of a one-dimensional random walk, with a diffu-
sivity proportional to the kink concentration. Assuming that the step is on average
aligned with the $x$-axis, the roughness can be quantified by the height-difference

$$\langle [y(x) - y(x')]^2 \rangle = \frac{k_B T}{\delta} |x - x'|.$$ (2.5)

Here the angular brackets refer to a thermal average with respect to the equilibrium
distribution. The relation (2.5) has been widely exploited to derive, via (2.4),
experimental estimates for the kink energy $\epsilon$ from scanning tunneling microscopy
observations of step fluctuations [7, 8].

A thermodynamic consequence of step roughness is that the step free energy
$\delta(\theta)$ cannot contain any singularities. Via the Wulff construction [1, 6], this implies
that the corresponding equilibrium island shapes have finite curvature everywhere
(compare to (2.3)), and hence display no corners or “facets” in the thermodynamic
limit (of course, islands of a size comparable to or smaller than the mean distance
between kinks nevertheless have atomically straight edges). This is in contrast to
the three-dimensional case, where cusps in the Wulff-plot of the surface free energy
lead to facets in the equilibrium crystal shape [6, 9].

2.3. Step-step interactions

So far we have considered a single atomic step in isolation. To understand the
thermodynamics and kinetics of stepped surfaces, which consist of an array of
parallel steps of equal sign (see Fig.4), it is crucial to take into account also the
interactions between the steps. An important source of interaction is the very fact that steps are thermally rough. As was first noted by Gruber and Mullins [10], in an array of parallel steps the thermal wandering of a given step is impeded by collisions with its neighbors (since the steps cannot cross). This reduces the entropy of the step, thus increasing its free energy and leading to an effective repulsion between the steps.

It is straightforward to estimate the strength of the repulsion from (2.5). Suppose the average distance between the steps (along the perpendicular y-direction) is \( l \). Then the collision length \( L_c \), the distance between close encounters of two steps measured along the parallel x-direction, is obtained by setting the left hand side of (2.5) equal to \( l^2 \) and inserting \( L_c \) for \(|x - x'|\). This yields \( L_c \approx \bar{\delta} l^2 / (k_B T) \). Assuming a fixed entropy loss \( k_B C \) per collision, the free energy of the step is then increased by an amount

\[
\Delta \delta \approx \frac{C k_B T}{L_c} = \frac{C (k_B T)^2}{\bar{\delta} l^2}.
\]

The coefficient \( C \) can be evaluated for a model in which the steps are represented as world lines of non-interacting fermions (subject only to the non-crossing constraint), which yields \( C = \pi^2/6 \) [11].

The important feature of (2.6) is that the step interactions decay quite slowly with step distance, as \( l^{-2} \). There is extensive experimental support for this interaction law from scanning tunneling microscopy measurements of the distribution of step spacings on vicinal surfaces [7, 8]. However, the interaction strength is typically found to be considerably larger than predicted by the purely entropic expression (2.6). This is because elastic interactions between the strain fields associated with the steps, mediated through the bulk crystal, display the same \( l^{-2} \) decay law, and typically dominate the entropic interactions. Electrostatic dipoles associated with the steps also lead to an \( l^{-2} \)-interaction. A macroscopic consequence of the \( l^{-2} \)-repulsion is the singular behavior \( z(y) - z(y_0) \sim (y - y_0)^{3/2} \) of the height of the equilibrium crystal shape \( z(y) \) near a facet edge at \( y = y_0 \) [5, 6, 9].

3. Step dynamics as a moving boundary problem

Within the step dynamical picture, a step is a mathematically sharp boundary that evolves by exchanging mass with the continuous adatom concentration field \( n(x, y, t) \) on the terraces. Thus the formulation of a step dynamical model requires, first, the specification of the dynamics of the adatom concentration, and, second, the formulation of boundary conditions for \( n \) at the steps. Whereas the first part is quite straightforward, the second contains a number of (explicit and implicit) assumptions about the underlying microscopic physics. As the formulation of the appropriate boundary conditions constitutes a central part of the step-dynamical modeling approach, we will discuss these issues in considerable detail.
3.1. Adatom dynamics
We want to describe physical situations where atoms arrive at the surface with a deposition flux $F$, diffuse over the terraces with a surface diffusion coefficient $D$, and possibly desorb back into the vacuum at rate $1/\tau$. In some cases it is also of interest to include a directed force $\vec{f}$ acting on the adatoms due to an electric current in the bulk of the sample (surface electromigration) [12, 13, 14]. Together these processes imply the evolution equation

$$\frac{\partial n}{\partial t} = D \nabla^2 n - D \frac{k_B T}{\tau} \vec{f} \cdot \nabla n + \frac{n}{\tau} = -\nabla \cdot \vec{J} + F - \frac{n}{\tau}$$  \hspace{1cm} (3.1)

for the adatom concentration field. Here the adatom current $\vec{J}$ has been introduced, which is generally driven by the concentration gradient as well as by the electromigration force. The coefficient $D/k_B T$ in front of the drift term is the adatom mobility, which is related to the diffusion coefficient through the Einstein relation.

The motion of the steps is often slow compared to the time scale on which the adatom concentration changes, so that (3.1) can be solved quasistatically, setting $\partial n/\partial t = 0$. To see when this approximation is justified, consider for concreteness the case of growth, and suppose that the typical distance between steps is $l$. Then the step velocity is of the order $v \sim F \Omega l$, which is to be compared to the diffusion velocity $v_D \sim D/l$, the effective speed of an atom diffusing over the distance $l$ [15]. The quasistatic approximation holds if $v \ll v_D$ or

$$l \ll \left( \frac{D}{\Omega F} \right)^{1/2}. \hspace{1cm} (3.2)$$

This condition is essentially always fulfilled, because nucleation of new islands creates steps at typical distances $l_D \sim (D/F)^{\chi}$, where $\chi < 1/2$ [4], and hence the step density is usually much larger than required according to (3.2). The situation is different in the presence of an electromigration force, because then also the drift velocity $v_{\text{drift}} = (D/k_B T)|\vec{f}|$ of the adatoms would be required to be large compared to $V$; since the electromigration force is very weak, this condition is not necessarily satisfied [16] (see also Sect. 3.8). In the following we nevertheless adhere to the quasistatic approximation.

3.2. Kinetic processes at the step
The interaction of adatoms with steps involves the following microscopic processes [17, 18, 19] (see Fig. 2):

- **Attachment and detachment.** It is important to note that these processes actually consist of two stages: When attaching to the step, an adatom first attaches to a straight step segment and then moves along the segment until it reaches a kink, where it is incorporated; similarly a detachment event requires first that an atom detaches from a kink to the straight step, and subsequently detaches from the step segment onto the terrace.
- **Step crossing.** The foregoing remark implies that an atom may also cross a step without attaching to a kink; this happens if the kink concentration is
low and the binding to the straight step weak, so that the step atom detaches from the straight step before a kink is encountered.

- **One-dimensional nucleation** \[20\]. If two step atoms are present simultaneously on a straight segment of the step, they can meet and form a step dimer, which is essentially a pair of kinks of opposite sign. This provides a nonequilibrium mechanism for the creation of kinks, in addition to the thermally excited kinks that are present in equilibrium (see Sect. 2.2). If step atoms cannot detach onto the terrace, the typical distance between kinks created by one-dimensional nucleation is

\[
l_{1d} \sim \left( \frac{D_e}{F_{1d}} \right)^{1/4},
\]

where \(D_e\) is the diffusion coefficient of a step atom along a straight step segment, and \(F_{1d}\) is the one-dimensional flux impinging onto the step from the terrace \[21, 22\]. Generalizations of (3.3) to other conditions can be found in \[17, 20, 23\].

- **Diffusion along a rough step.** Since steps always contain a finite concentration of kinks (of equilibrium or nonequilibrium origin), mass transport by step edge diffusion requires that step atoms are able to cross kinks and corners. The diffusion along a rough step is therefore considerably slower than the diffusion along a straight step segment. As indicated in Fig. 2, a step atom crossing a kink “from above” first has to round the kink and then detach from it onto the step. Kink rounding is often associated with an additional energy barrier \([24, 25, 26]\).

![Diagram of atomic processes at a step: Attachment (A) and detachment (D) of terrace atoms; step crossing (SC); kink crossing (KC); and one-dimensional nucleation (1DN). As in Fig. 1, the upper terrace is shaded.](image)

**Figure 2.** Atomic processes at a step: Attachment (A) and detachment (D) of terrace atoms; step crossing (SC); kink crossing (KC); and one-dimensional nucleation (1DN). As in Fig. 1, the upper terrace is shaded.

### 3.3. Linear constitutive relations

Within the step dynamical model, the diverse and rather complex processes described in the preceding subsection are lumped together into the net mass currents \(j_+\) and \(j_-\) from the lower and upper terrace, respectively, and the edge diffusion
current $j_e$ (see Fig. 1). In the spirit of linear nonequilibrium thermodynamics, these currents are assumed to be linear in the adatom concentration gradients and differences. Consider first the edge diffusion current $j_e$, which counts the number of atoms that pass a point on the step in unit time. It is of the form

$$ j_e = -\sigma \frac{\partial \mu}{\partial s}, $$

(3.4)
a relation that can be taken to define the mobility $\sigma$ of an edge atom along a (rough, curved) step [26, 27]. It is important to keep in mind that (3.4) includes only that part of the mass transport along the step that is induced by differences in the step chemical potential, and hence serves to restore thermal equilibrium at the step. In addition, there are genuinely nonequilibrium contributions to the current that arise from the combined effects of attachment, step edge diffusion and kink rounding barriers [24, 25, 28, 29].

**Figure 3.** Behavior of the adatom concentration near a step.

Figure 3 illustrates how the adatom concentration changes across a step. At each point of the step, three different values of $n$ can be defined: The limiting value $n_+$ ($n_-$) attained by the terrace concentration field $n(x, y)$ when approaching the step from the lower (upper) terrace, and the equilibrium step atom concentration $n_{eq}$ which would be established in the absence of growth, through the detachment of atoms from thermally excited kinks. The mass currents $j_+$ and $j_-$ that leave a terrace via the ascending and descending step, respectively, are now written as linear combinations of the differences between these adatom concentrations, in the form (see e.g. [16])

$$ j_+ = k_+(n_+ - n_{eq}) + p(n_+ - n_-) $$

(3.5)
and

$$ j_- = k_-(n_- - n_{eq}) - p(n_+ - n_-). $$

(3.6)
The first term on the right hand side of (3.5) is the net current of terrace atoms that attach to the step from below, while the second term is the current of atoms that cross the step without attaching to it. The first contribution is driven by
the deviation of the adatom concentration from its equilibrium value, while the second contribution is driven by the difference of the adatom concentrations on the two terraces. Similar considerations apply to the current (3.6) from the upper terrace. The kinetic coefficients $k_+$ and $k_-$ are known as attachment rates, while the coefficient $p$ is referred to as the step permeability; see Sects. 3.6 and 3.7 for further discussion of physical effects related to these quantities. Usually all kinetic coefficients are assumed to be positive, but negative values can also be meaningful under certain conditions [30] (see Sect. 4.3). The symmetry between the step crossing terms in (3.5) and (3.6) can be viewed as a consequence of the Onsager reciprocity relations [16].

The linearity of the constitutive relations (3.4, 3.5, 3.6) contains the implicit assumption that the step is close to equilibrium. There have been recent attempts to formulate kinetic models that do not require this assumption [18, 19], but the bulk of the work in the field relies on it. Detailed kinetic modeling is also needed to derive expressions for $k_\pm$ and $p$ in terms of the rates of elementary atomic processes. Here we follow the common practice and regard the kinetic coefficients in (3.5, 3.6) as phenomenological parameters.

3.4. Thermodynamic driving force

The thermodynamic driving forces that are responsible for restoring equilibrium enter (3.4) through the equilibrium adatom concentration $n_{eq}$, which is related to the (local) step chemical potential through the standard thermodynamic identity

$$n_{eq} = n_{eq}^0 e^{\mu/k_BT} \approx n_{eq}^0 (1 + \mu/k_BT).$$  \hspace{1cm} (3.7)

Here $n_{eq}^0$ is the equilibrium adatom concentration at an isolated, straight step, and the second relation assumes that the deviations from this value are small. As was discussed in Sect. 2, the step chemical potential is affected by the step curvature [see (2.2)] and by the step-step interactions. To derive the latter contribution, we denote by $y_j(x)$ the position of the $j$-th step in the $(x,y)$-plane, and assume (following Sect. 2.3) that the free energy of the step-step interaction (including both entropic and direct, elastic or electrostatic contributions) for two steps at a distance $l$ is of the form $V(l) = A/l^2$, where $A$ is the interaction strength. Then the contribution to the step chemical potential of step $j$ from the interaction with the neighboring steps $j-1$ and $j+1$ is

$$\Delta \mu_j^{int} = \frac{\partial}{\partial y_j} [V(y_{j+1} - y_j) + V(y_j - y_{j-1})]$$  \hspace{1cm} (3.8)

and together with the curvature contribution the expression for the chemical potential of step $j$, to be inserted in (3.4), is

$$\mu_j = \Omega \delta \kappa_j + 2A \left[ \frac{1}{(y_{j+1} - y_j)^2} - \frac{1}{(y_j - y_{j-1})^2} \right],$$  \hspace{1cm} (3.9)

Footnote: For the step edge mobility $\sigma$ in (3.4) such a derivation has been achieved, see [20, 27].
with \( \kappa_j \) denoting the curvature of step \( j \). Note that all terms in (3.9) also depend on the coordinate \( x \) along the step.

### 3.5. Mass conservation

Once the mass currents \( j_\pm \) have been fixed through the constitutive relations (3.5, 3.6), the boundary conditions for the adatom concentration field as well as the evolution equations for the step follow simply from mass conservation. This requires, first, that the mass currents are continuous at the step, which means that the total terrace current \( \vec{J} \) appearing on the right hand side of (3.1) must be matched to the local currents \( j_\pm \) at the steps. Thus

\[
j_+ = D \vec{n} \cdot \left[ \nabla n|_+ - \frac{1}{k_B T} \vec{f}_n \right]
\]

and

\[
j_- = -D \vec{n} \cdot \left[ \nabla n|_- - \frac{1}{k_B T} \vec{f}_n \right],
\]

where \( \nabla n|_\pm \) are the values of the concentration gradient on the two sides of the step, and \( \vec{n} \) is the unit vector normal to the step, which points towards the lower terrace. Together with (3.5, 3.6), these equations constitute the boundary conditions for the solution of the (quasistatic) drift-diffusion equation for \( n \).

The second consequence of mass balance is that the step moves in response to the net attachment current \( j_+ + j_- \) (note that the contributions due to step crossing cancel), as well as due to the mass transport along the step. The normal velocity of the step is therefore given by

\[
v_n = \Omega \left( j_+ + j_- - \frac{\partial j_e}{\partial s} \right).
\]

This completes the derivation of the step-dynamical model.

### 3.6. The Ehrlich-Schwoebel effect

The attachment rates \( k_\pm \) were introduced by Schwoebel in his seminal 1969 paper [31]. Schwoebel and Shipsey were the first to explore the consequences of attachment asymmetry (\( k_+ \neq k_- \)) for the stability of growing stepped surfaces [31, 32]. Their work was triggered by the field ion microscope observation of Ehrlich and Hudda that tungsten adatoms on tungsten surfaces tend to be reflected by descending step edges [33], which implies that \( k_+ < k_- \). Therefore the preferential attachment to ascending steps, which is observed for many materials, is often referred to as the (normal) Ehrlich-Schwoebel (ES) effect.

For metal surfaces, the ubiquity of the normal ES effect is now fairly well established [1], but for semiconductor materials the situation is less clear. For example, for the Si(111)-surface, a detailed microscopy study of island nucleation near steps [34] provides evidence for an inverse ES effect (\( k_+ < k_- \)) at high temperatures, above the transition from the \((7 \times 7)\) to the \((1 \times 1)\) reconstruction, but at lower temperatures (below the transition) a study of electromigration-induced step and island motion [35] indicates that, on the contrary, \( k_+ > k_- \).
3.7. Step permeability

The importance of step crossing processes for the evolution of the surface morphology has been realized only fairly recently. Step permeability in the sense of (3.5, 3.6) was first introduced in 1992 by Ozdemir and Zangwill [36]. The dimensionless ratio $p/k_\pm$, which is a measure for the probability that an atom crosses the step without being incorporated, can be quite large for semiconductor surfaces, where the incorporation process may be difficult because of reconstructions at the step. From an analysis of the relaxation of biperiodic gratings on Si(001) it was concluded that $p/k_\pm = 40 \pm 20$ for this system [37]. But also steps on metal surfaces can be highly permeable, as evidenced by the dramatic formation of steep pyramids on Al(110) [38], which cannot be explained without substantial transport across steps. In the fully permeable limit, $p \to \infty$, the finiteness of the current in (3.5, 3.6) forces the adatom concentration to be continuous at the steps. Some consequences of step permeability will be described in Sect. 4.3.

3.8. Kinetic lengths

Inserting the expressions (3.5) and (3.6) on the right hand sides of (3.10) and (3.11), the boundary conditions are seen to identify gradients of the adatom concentration $n$, multiplied by $D$, with differences in $n$, multiplied by kinetic coefficients. As a consequence, the ratios of $D$ to the kinetic coefficients naturally define the length scales

$$l_+ = \frac{D}{k_+}, \quad l_- = \frac{D}{k_-}, \quad l_0 = \frac{D}{p},$$

(3.13)

which are collectively referred to as kinetic lengths. The kinetic lengths are useful in discussing the effects of step boundary conditions on the morphological evolution. For example, in assessing the importance of a conventional ES effect in growth, it is crucial to compare the typical terrace sizes to the kinetic length $l_-; the ES effect is strong, and makes itself felt during the growth of the first few layers, if $l_-$ is large compared to the terrace size [3, 4] (see also Sect 4.1.1). Similarly the comparison of the two terms inside the square brackets in (3.10) and (3.11) leads to the definition of the electromigration length [39]

$$\xi = \frac{k_B T}{|f|},$$

(3.14)

and the discussion of non-quasistatic effects can be phrased in terms of a “Péclet-length”

$$\xi_P = \frac{D}{v},$$

(3.15)

where $v$ is the step velocity [16]. This is motivated by the fact that going to a frame moving with speed $v$ introduces a convection term $v \nabla n$ in the stationary diffusion equation, which is of the same form as the electromigration term in (3.1). In general, the quasistatic approximation requires that all other relevant length scales are small compared to $\xi_P$. 
4. Morphological stability

The solution of the moving boundary problem formulated in the preceding section in its full generality is a formidable challenge. For this reason much of the work in this area has been restricted to linear stability analyses of simple surface morphologies. The most important results will be summarized in this section.

4.1. Stability of growing and sublimating step trains

The basic instability modes of a regular step train—a vicinal surface with straight, equidistant steps—are illustrated in Fig. 4: Either the surface separates into regions of high step density (step bunches) and wide terraces, or the steps become wavy (step meandering). While the two modes are usually assumed to be mutually exclusive, there is experimental evidence from homoepitaxial growth that they may also coexist \[40, 41\].

4.1.1. Bunching of straight steps.

The stability analysis is particularly simple if the steps can be assumed to remain straight, because then the dynamical problem reduces to a set of ordinary differential equations coupled along the \( y \)-direction. The basic stability results for straight, impermeable steps were derived by Schwoebel and Shipsey \[31, 32\], who showed that a growing step train is stabilized by a normal ES effect \( (k_+ > k_-) \) while the same effect leads to step bunching during sublimation; conversely, an inverse ES effect \( (k_+ < k_-) \) implies step bunching during growth. Explicitly, the equations of motion for the step positions \( y_j \) during growth are of the form

\[
\frac{dy_j}{dt} = f_+(y_{j+1} - y_j) + f_-(y_j - y_{j-1}),
\]  

Figure 4. Instability modes of a vicinal surface.
where $f_+$ and $f_-$ denote the contributions from the leading and the trailing terrace, respectively, which are given by

$$f_{\pm}(l) = \frac{F\Omega l}{2} \left( \frac{2l_{\pm} + l}{l_{\pm} + l + l} \right).$$

(4.2)

Here the effects of step-step interactions arising from the step chemical potential have been neglected. A straightforward linear stability analysis of (4.1) shows that the equidistant step train is stable provided $d[f_+(l) - f_-(l)]/dl > 0$, which, using the explicit expression (4.2), is seen to be equivalent to $k_+ > k_-$. The functional form of (4.2) illustrates the role of the kinetic lengths $l_{\pm}$ in gauging the strength of the attachment asymmetry: When the terrace size $l \gg l_{\pm}$ the attachment kinetics becomes effectively symmetric and $f_+ \approx f_- \approx F\Omega l/2$.

![Figure 5](image)

**Figure 5.** Stabilization of a configuration of equidistant, straight steps by a normal ES effect. Step $j$ receives most of its flux from the leading terrace $y_j < y < y_{j+1}$. It therefore moves faster than the neighboring steps, and the step spacing is equalized. In our notation the terrace in front of step $j$, measured from an arbitrary reference level, is at height $h = -aj$, where $a$ is the (vertical) lattice constant.

The stabilization of the growing step train by the normal ES effect is illustrated in Fig.5. Formally it can be interpreted in terms of an effective step-step repulsion mediated by the diffusion field on the terraces. This repulsion is very efficient, in the sense that it leads to terrace width fluctuations that are much smaller than the corresponding fluctuations in thermal equilibrium [42, 43].

The fact that a normal ES effect stabilizes the regular step spacing implies that step bunching during growth – which is actually observed rather frequently in experiments – requires a separate mechanism for its explanation. It has been realized for a long time that impurities may cause step bunching during growth [44, 45, 55]. Recently it was pointed out by Pimpinelli and coworkers that step bunching can also be induced if the diffusing species that is incorporated during growth (e.g., the adatoms) is coupled to a second species, which could be a
chemical precursor in the case of chemical vapor deposition [47] or highly mobile dimers [48]. Using a two-species generalization of BCF theory, it can be shown that under suitable conditions a normal ES effect for the second species implies an effective inverse ES effect for the growth species, and hence causes step bunching. On reconstructed surfaces such as Si(001) the pronounced anisotropy of terrace diffusion can also cause step bunching [49]. Finally, through a subtle coupling to a preceding meandering instability, fast edge diffusion has been predicted to provide a mechanism for step bunching [28]. This last scenario seems consistent with the combined meandering and bunching instability observed for Cu(100) [40, 41].

4.1.2. Step meandering. Bales and Zangwill (BZ) first showed that a normal ES effect induces step meandering during growth [50]. Because of the effective step-step repulsion, the meander can be most easily accommodated if the steps meander in phase, as indicated in Fig. 4. Within the linear stability analysis, this implies that the in-phase meander is the mode with the largest growth rate [51]. A fundamental result of the BZ analysis is a prediction for the meander wavelength in the initial stage of the instability. In the absence of desorption but taking into account edge diffusion, the relevant expression reads

$$\lambda_{BZ} = 4\pi \sqrt{\frac{D^{\text{eq}} l}{k_B T + \sigma} \frac{\Omega \delta f_{\text{ES}}}{F l^2 f_{\text{ES}}}}. \tag{4.3}$$

Here \(l\) is the step spacing of the vicinal surface, which is assumed to be small compared to the meander wavelength, and the factor \(f_{\text{ES}} = (l_+ - l_-)/(l_+ + l_- + l) > 0\) is a measure for the strength of the ES effect. Equation (4.3) makes it clear that the meander wavelength is determined by the competition between the destabilizing flux in the denominator, and the stabilizing thermodynamic forces represented by the step stiffness in the numerator; shifting the balance towards the stabilizing/destabilizing side increases/decreases the meander wavelength. The stiffness is multiplied by the sum of two kinetic coefficients representing the two kinetic pathways that contribute to smoothening the step, terrace diffusion and step edge diffusion.

The basic mechanism underlying the BZ instability is well known from more conventional diffusional interface instabilities, e.g. in solidification [52]: The preferential attachment of adatoms to the ascending step implies that the growth of protrusions in the step is amplified. In contrast to solidification, however, here we are dealing with an infinite array of coupled “interfaces”. The situation is illustrated in Fig. 5. It is clear from this figure that the essential feature needed for the instability is that the flux reaching the step from the lower terrace is larger than the corresponding flux from the upper terrace. Such an imbalance can be achieved even without an attachment asymmetry, by simply making the lower terrace larger than the upper terrace. Experiments on suitably tailored step structures on the Si(111) surface [50] (for which the existence of a ES effect is controversial, see Sect. 3.6) do indeed produce meander patterns, and confirm the prediction of the BZ linear stability analysis that the meander wavelength should scale with the
Figure 6. Geometric origin of the Bales-Zangwill meandering instability [54, 55]. The terraces are subdivided into lots along the dotted lines, which are drawn perpendicular to the lines of constant adatom concentration. Each lot receives the same number of atoms per unit time, which, owing to the ES effect, attach primarily to the corresponding segment of the ascending step. Because of the meander, the indented segments of the step are longer than the protruding ones. Since both receive the same total flux, the protrusions propagate faster and the meander is amplified.

inverse square root of the flux [see (4.3)]. By the same argument, step meandering can result if the upper and lower terraces differ, e.g., in the diffusion or desorption rates for adatoms, a situation that is relevant to growth on Si(111) near the $7 \times 7 \rightarrow 1 \times 1$ transition temperature [57].

A detailed experimental study of the temperature and flux dependence of the meander wavelength was reported recently for growing surfaces vicinal to Cu(100) [41, 58, 59]. The main conclusion of this work was that the experimentally observed meander instability cannot be attributed to the BZ mechanism; instead, it seems that quantitative agreement can be reached [23, 60] if an alternative mechanism associated with kink rounding barriers (the Kink Ehrlich Schwoebel Effect or KESE) [24, 25, 28] is assumed to be operative. The KESE is the one-dimensional analog of the ES effect [41]. In the present case it is triggered by the disturbances created by one-dimensional nucleation events on the perfectly straight steps. Consequently the initial meander wavelength is given by the nucleation length (3.3). This changes the exponent of the flux dependence as compared to (4.3), and leads to a temperature dependence governed by the activation energy for step edge diffusion.

In contrast to the BZ instability, the KESE acts independently at each step, and hence there is no specific phase relation between the deformations of different steps in the initial regime of the instability [23]. Phase coherence develops later due
to the effective step-step repulsion induced by the ES effect or, in the absence of any attachment asymmetry, due to entropic or energetic step interactions; particularly in the last case, the synchronization of the step meanders is found in simulations to be very slow [61].

Step meandering can also occur in the absence of either a ES effect or a KESE, if edge diffusion is sufficiently fast. The phenomenon was discovered in kinetic Monte Carlo simulations [25], and it can be understood within the framework of a coarse grained continuum ("height") description of the surface, based on the notion of growth-induced surface currents [3, 4, 62, 63] (see also Sect 5). The starting point of the height description is a suitable phenomenological nonlinear partial differential equation for the surface height field \( h(x, y, t) \). The stability analysis for a growing vicinal surface carried out in this setting shows that the surface is unstable towards step meandering whenever there is a net surface current in the uphill direction [27, 64]. Such a current can be argued to arise by step edge diffusion for purely geometric reasons, if the steps are already somewhat wavy; then the motion of an atom along a step, directed on average from protrusions to indentations, also has an uphill component. Because it presupposes a certain step corrugation, the effect is, in a sense, nonlinear, and it has so far not been possible to treat it within the conventional stability analysis of the step dynamical model. Kinetic Monte Carlo simulations indicate that the meander wavelength scales with flux as \( \lambda \sim F^{-1/4} \), but a theoretical understanding of this result is lacking [65].

4.2. Stability of islands

We have emphasized in the preceding subsection that the BZ instability requires a larger flux to the step from the lower, compared to the upper, terrace. It is clear that this situation also arises during the growth of two-dimensional islands on a singular surface (a surface without preexisting steps). When the islands nucleate their radius is much smaller than the distance between islands [2, 4], and hence the adatoms that contribute to the growth of the island originate mainly from the substrate, i.e. from the lower terrace relative to the island boundary. Conversely, in the late stage of growth close to island coalescence, the island boundary is mainly fed from above, as the uncovered areas between islands are smaller than the islands themselves. One therefore expects that the island boundary should be unstable to meandering during the early stages of growth, and that it is restabilized when coalescence is approached. Of course it is also possible that the island boundary remains stable, if the island size is small compared to the characteristic meander wavelength [given e.g. by (4.3)] throughout the growth history.

This qualitative picture is confirmed by linear stability analyses. The first study of island stability was carried out by Avignon and Chakraverty, who considered a single island growing in the presence of desorption [30]; in this case the length scale for the island size at which restabilization sets in is given by the diffusion length

\[
x_s = \sqrt{D\tau},
\]

(4.4)
which is a measure for the range of correlations induced by the diffusion field. The first mode that becomes unstable during growth is a deformation of threefold symmetry\(^2\). A self-consistent treatment of island stability in the presence of surrounding islands was performed by Bales and Chrzan \[67\], who arrived at similar conclusions. Initial instability followed by restabilization has been observed experimentally for micron-sized islands on Si(111) \[56\].

4.3. Stability under surface electromigration

In 1989, Latyshev and collaborators reported that a direct heating current can induce step bunching on surfaces vicinal to Si(111) \[68\]. The bunches dissolve upon reversing the current direction, which suggested the hypothesis \[12\] that a current-driven directed motion of silicon adatoms – *surface electromigration* – may be responsible for the phenomenon\(^3\). In a seminal paper, Stoyanov included the electromigration force into the BCF theory and showed that step bunching indeed occurs, if the force is in the down-step direction \[70\]. Subsequent experimental work has confirmed the electromigration hypothesis, but at the same time a bewildering diversity of electromigration-induced patterns on vicinal silicon surfaces has been discovered \[13, 14\].

In particular, the current direction needed to induce step bunching was found to reverse three (!) times with increasing temperature. The scenario first proposed by Stoyanov \[70\] appears to apply to the lowest temperature regime (regime I), and much theoretical work has been devoted to trying to understand the reversals at higher temperatures. The simple idea that the reversals may be attributed to a sign change of the effective charge of the adatoms \[71\] has been ruled out by experiments \[72\] which show that the direction of the force coincides with the current direction at all temperatures. Other mechanisms that have been proposed to explain the reversals include strong desorption, in the sense that the diffusion length \[4.4\] becomes comparable to the step spacing \[70\], and diffusion and drift of surface vacancies \[73\].

While the issue is far from being settled, recent work seems to converge on the view that the resolution of the puzzle must be sought in the boundary conditions for the adatom concentration, at least as far as the first reversal (from regime I to regime II) is concerned. Stoyanov first showed that step bunching occurs, in the presence of sublimation, for a force in the up-step direction, if the steps are assumed to be perfectly permeable \((l_0 = 0\) in \(3.13\)) \[74, 75\]. Moreover, he predicted that the unstable current direction should reverse in the presence of a growth flux, in agreement with subsequent experiments \[76\]: at least in the absence of an attachment asymmetry, no such dependence on growth or sublimation conditions is present for impermeable steps \[16\]. Further support for the permeability picture comes from the observation of in-phase step meandering in regime II, when the current is in the down-step direction \[77\], a phenomenon that is reproduced by the linear stability analysis for permeable steps \[78\].

\(^2\)Crystal anisotropy of the stiffness or the kinetic coefficients is not taken into account in \[66, 67\].

\(^3\)For a general discussion of electromigration effects see \[69\] and references therein.
Nevertheless alternative explanations cannot be ruled out. For example, it has been argued that the consequences of fast attachment kinetics, in the sense of \( l_+ l_- \ll l \), can hardly be distinguished from those of step permeability \[16\]. Evidence for step bunching due to an uphill force in the case of fast attachment kinetics has been found in kinetic Monte Carlo simulations, and the effect has been reproduced in a linear stability analysis assuming an electric field dependence of the kinetic coefficients and the equilibrium adatom concentration in the boundary conditions \[8, 30, 74\]. A particularly elegant recently proposed scenario for the stability reversal is based on the observation that the effective kinetic coefficients \( k_\pm \) entering the boundary conditions may become negative, if the step is treated as a spatially extended region in which the diffusion of adatoms is enhanced rather than hindered relative to diffusion on the terraces \[30\]. Indeed, noting that the basic stability criterion derived by Stoyanov in his 1991 paper \[70\] involves the product of the electromigration force and the attachment coefficient, it is clear that a sign reversal of the kinetic coefficient is tantamount to a reversal of the direction of the force.

Additional complications, not discussed here, arise when the current direction is varied continuously relative to the orientation of the steps \[62, 80, 81\].

5. Nonlinear evolution

5.1. Step bunching

Numerical integration of the step dynamical equations in the nonlinear regime has been largely restricted to the bunching of straight steps, where the problem reduces to a one-dimensional array of coupled ordinary differential equations; representative examples out of a large number of publications are \[82, 83, 84, 85\]. The main interest in these studies has been to characterize the shape of individual bunches, as well as the time evolution of the typical bunch size due to bunch coarsening and coalescence. For both aspects quantitative information is available from experiments on electromigration-induced step bunching of surfaces vicinal to Si(111) \[86, 87, 88\].

Some of the bunch properties can be derived analytically by passing from the discrete step dynamics to a continuum description of the one-dimensional height profile \( h(y, t) \) perpendicular to the steps \[62\]. The continuum limit is rather straightforward for the case of step flow growth, because the creation and annihilation of steps by island nucleation and coalescence does not have to be taken into account. We sketch the derivation for a particularly simple situation, thus providing an illustration of how the step dynamical model can be related to the continuum height equations discussed elsewhere in this volume \[63\].

Specifically, consider step bunching in the regime of a strong inverse ES effect, such that the typical step spacing \( l \) satisfies \( l_+ \gg l \gg l_- \). Then the equations of
motion (4.1, 4.2) become linear,

$$\frac{dy_j}{dt} = \hat{F}(y_j - y_{j-1}),$$

(5.1)

where $\hat{F} = F \Omega$. Clearly $y_j(t)$ can be replaced by a continuous function $y(h,t)$, where $h = -aj$ (compare to Fig.5), by simply expanding the difference on the right hand side of (5.1). To second order this yields

$$\frac{\partial y}{\partial t} = \hat{F} \left[-a \frac{\partial y}{\partial h} - \frac{a^2 \partial^2 y}{\partial h^2}\right].$$

(5.2)

Applying the chain rule in the form

$$\frac{\partial h}{\partial t} = -\frac{\partial h}{\partial y} \frac{\partial y}{\partial t},$$

(5.3)

appropriate for the negatively sloped surface, we obtain a nonlinear evolution equation for $h(y,t)$ [89],

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial y} \left[-\hat{F}a \left(\frac{\partial h}{\partial y}\right)^{-1}\right] = \hat{F}a.$$

(5.4)

The right hand side of this equation is naturally interpreted as a conservation law with a *growth-induced current* [3, 4, 55, 62, 63], which is inversely proportional to the surface slope and directed downhill (recall that $\partial h/\partial y < 0$).

The step-step interaction terms arising from (3.9) can be handled in a similar way [90]. Putting together the destabilizing and stabilizing effects, the resulting surface evolution equation takes the general form

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial y} \left[-A \left(\frac{\partial h}{\partial y}\right)^{-1} + B \left(\frac{\partial h}{\partial y}\right)^{-1} \frac{\partial^2}{\partial y^2} \left(\frac{\partial h}{\partial y}\right)^2\right] = \text{const.}$$

(5.5)

where the coefficients $A$ and $B$ are positive, and the constant on the right hand side is the deposition flux. The same evolution equation has been obtained for step bunching induced by a normal ES effect during sublimation [62] and for electromigration-induced step bunching in the limit of slow attachment/detachment kinetics ($l_\pm \gg l_\infty$) [83]. It applies whenever the destabilizing part of the step dynamical equations, which is responsible for the step bunching instability, becomes linear in the step spacings [as in (5.1)].

The scaling properties of stationary step bunches can be derived from (5.5) by setting the current inside the square brackets to a constant and investigating the resulting ordinary differential equation for the slope $\partial h/\partial y$ [83, 89, 91]. One finds, in particular, that the minimal terrace size $l_{\min}$ inside the step bunch (the inverse of the maximal slope) scales with the number of steps $N$ in the bunch as $l_{\min} \sim N^{-2/3}$, which is close to the behavior observed in experiments [57, 88]. At present it is not clear to what extent continuum equations like (5.5) are capable of also describing the time-dependent behavior of step bunches [82].

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4The expansion has to be carried to third order in the symmetric case $k_+ = k_-$. [89].
Equation (5.5) is a representative of a larger class of evolution equations which have been proposed within a general classification scheme for step bunching phenomena. All these equations are highly nonlinear, in the sense that the typical nonlinearities have the form of inverse powers of the slope. A different kind of evolution equations with polynomial nonlinearities arises when the derivation is carried out close to the threshold of the step bunching instability.

Finally, we note that all continuum equations discussed so far in this subsection have the form of a local conservation law [broken only by a constant flux on the right hand side, see (5.4) and (5.5)]. One might expect that this reflects the absence of desorption from the surface, which generally violates the property of volume (hence height) conservation. However, the explicit derivation of an equation of the form (5.5) for sublimation-induced step bunching shows that the structure of the conservation law is retained even in this case, provided desorption is a weak effect, in the sense of the diffusion length being large compared to the other relevant length scales. In the presence of strong desorption one obtains instead an evolution equation with polynomial singularities of Kuramoto-Sivashinsky type, which displays spatiotemporal chaos rather than coarsening behavior (see [62] for a general discussion).

5.2. Step meandering

The nonlinear evolution of growth-induced step meandering has been studied mostly within the framework of local approximations to the nonlocal moving boundary problem, which can be systematically derived using multiscale techniques. The result of such a calculation is a one-dimensional, nonlinear partial differential equation which (depending on the situation of interest) describes either a single step interacting with the diffusion field or the collective step coordinate of a step train with an in-phase meander. As in the preceding subsection, evolution equations of nonconserved type (displaying spatiotemporal chaos) and conserved type may be distinguished. To give an example of the latter kind, the evolution equation

$$\frac{\partial y}{\partial t} = -\frac{\partial}{\partial x} \left\{ \frac{\alpha y_x}{1 + y_x^2} + \frac{\beta}{(1 + y_x^2)^\nu} \frac{\partial}{\partial x} \left[ \frac{y_{xx}}{(1 + y_x^2)^{3/2}} \right] \right\}$$

(5.6)

with positive coefficients $\alpha$, $\beta$ describes the collective step meander for the Bales-Zangwill instability; the exponent $\nu$ depends on whether the dominant step smoothing mechanism is terrace diffusion ($\nu = 1$) or step edge diffusion ($\nu = 1/2$). In both cases the equation displays unbounded amplitude growth, with $\langle y \rangle \sim t^{1/2}$, while the lateral wavelength of the pattern remains fixed. Related equations with other nonlinear terms may also display unbounded lateral coarsening or interrupted coarsening limited to a finite time interval (see also [62]).
6. Open problems

At the end of these introductory notes, it seems appropriate to formulate some open questions that could be, and should be, addressed in the near future.

6.1. Microscopic basis of kinetic coefficients

For the step dynamical model to attain predictive power, it is mandatory to achieve a good understanding of the relationship between the kinetic coefficients entering the boundary conditions and the underlying atomistic rates. There has been encouraging progress in this direction (see e.g. [23]), but the problem is clearly not solved in full generality. Presumably it will be necessary to go beyond the assumption of equilibrium at the steps, along the lines of [18, 19].

6.2. Crystal anisotropy

In the same vein, it is essential to take account of the fact that both thermodynamic and kinetic properties of steps on crystal surfaces are generally strongly anisotropic; still crystal anisotropy is ignored in most of the work in the field. As was recently demonstrated for the case of step meandering, anisotropy may qualitatively alter the evolution of morphological instabilities [101]. An attractive application for a numerical step-dynamical scheme incorporating crystal anisotropy would be to reproduce the sequence of island shapes that is observed experimentally as a function of temperature on metal surfaces such as Pt(111) [1].

6.3. Exotic step instabilities

We have briefly mentioned two novel step instabilities related to edge diffusion, which cannot be captured by straightforward linear stability analysis, and which thus may be termed exotic: The meandering instability caused by fast edge diffusion without attachment asymmetry or kink rounding barriers [25], and the step bunching instability induced by edge diffusion on steps with a preexisting meander [28]. So far evidence for the existence of these instabilities comes mainly from kinetic Monte Carlo simulations [25, 65]. A fully nonlinear treatment within the step dynamical model (including, in particular, the appropriate edge diffusion currents) would provide important guidance towards an analytic understanding, which is ultimately needed to assess the relevance of these effects for real surfaces.

6.4. Synchronization of the step meander

As was discussed above in Sect. 5.2, the nonlinear evolution of the step meandering instability has so far been treated under the assumption that the in-phase meander is fully coherent, so that the whole pattern can be described by a single step conformation \( y(x, t) \). With the availability of powerful numerical algorithm for the solution of the full moving boundary problem for multiple steps, it will soon be possible to address also the initial phase of the instability, where the phase relation between different steps is established. Gaining a better understanding of the synchronization process is important, because the phase defects in the meander pattern have been shown to act as seeds for secondary instabilities which eventually
lead to the proliferation of steps of a sign opposite to the initial vicinality, and hence to the breakdown of step flow \[64,102\]. Kinetic Monte Carlo simulations indicate that the breakdown is mediated by the formation of closed step loops deep in the fjords of the meander \[102\]. To handle such topology changes within the step dynamical model will require the use of approaches that avoid explicit tracking of the steps, such as phase field or level set methods, which are described elsewhere in this volume.

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