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Self-organization on surfaces/Auto-organisation sur les surfaces

# Dynamics of crystal steps

Olivier Pierre-Louis

*Laboratoire de spectrométrie physique, 140, avenue de la physique, BP 87, 38402 Saint Martin d'Hères, France*

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## Abstract

In this article, we wish to point out some of the recent advances in the study of step dynamics on crystal surfaces. We will first list some approaches to steps dynamics, based on irreversible thermodynamics, kinetic roughening concepts, and mass transport mechanisms. In a second part, we shall analyze step motion coupled to the diffusion of mobile atoms on terraces. A special focus will be given on pattern formation on vicinal surfaces and two-dimensional islands. Finally, we will report on the consequences of elastic and electronic relaxation on the dynamics of steps and adatoms. *To cite this article: O. Pierre-Louis, C. R. Physique 6 (2005).*

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## Résumé

**Dynamique des marches atomiques.** Nous présentons quelques avancées récentes dans l'étude de la dynamique des marches cristallines. Nous mentionnerons tout d'abord différentes approches pour la modélisation de la dynamique des marches, basées sur la thermodynamique des processus irréversibles, les théories de rugosification, et le transport de masse. Dans une deuxième partie, nous analyserons le mouvement de marches couplées à la diffusion des atomes mobiles à la surface. Nous développerons particulièrement le cas des surfaces vicinales et des îlots bidimensionnels. Finalement, nous étudierons les conséquences de la relaxation élastique et électronique du solide sur la dynamique des marches et des adatoms. *Pour citer cet article : O. Pierre-Louis, C. R. Physique 6 (2005).*

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## 1. What is a step?

### 1.1. Steps, terraces and adatoms

When one looks at a crystal at small scales during growth, the first surprising observation is that growth usually proceeds via the lateral flow of atomic steps (see Fig. 1). Rather than sticking to the crystal at the place where they have landed, atoms indeed diffuse until they attach to a step, thereby leading to the forward motion of steps. As reported in the work of Burton, Cabrera and Frank in 1951, the analysis of crystal growth can therefore be based on the analysis of step motion. Following this work,

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*E-mail address:* [olivier.pierre-louis@ujf-grenoble.fr](mailto:olivier.pierre-louis@ujf-grenoble.fr) (O. Pierre-Louis).

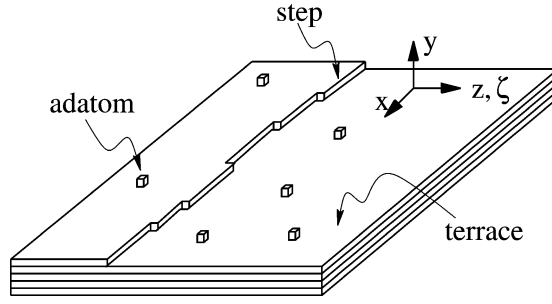


Fig. 1. Monoatomic crystal step, terrace, and adatom.

step motion has been widely studied to understand the formation of patterns at the nanometer and micrometer scales. In this review, we wish to present some of the recent advances in the analysis of step motion. More specifically, three questions will be our main focus: (i) What are the equations of motion and the structure of steps in non-equilibrium conditions, and at small scales? (ii) What are the patterns that are induced by step motion? (iii) What are the interactions between steps and atoms?

These three questions are the keys to the understanding of nanostructure formation, as a result of the nonlinear dynamics of fronts in non-equilibrium conditions, and involving long range interactions.

### 1.2. Burton–Cabrera–Frank model

Following the famous work of Burton Cabrera and Frank [1], we shall first model step kinetics in a macroscopic and phenomenological fashion, i.e. without referring to the underlying discreteness.

At the steps, mass conservation imposes:

$$\left(\frac{1}{\Omega} + c_- - c_+\right)V_n = -D\mathbf{n} \cdot \nabla c_- + D\mathbf{n} \cdot \nabla c_+, \quad (1)$$

where  $V_n$  is the normal step velocity,  $\pm$  respectively denote the upper and lower sides of the steps,  $D$  is the diffusion of mobile atoms on terraces,  $c$  is their concentration, and  $\Omega$  is the atomic area. On terraces (between the steps), we have, for example, during growth or sublimation:

$$\partial_t c = D\nabla^2 c + F - \frac{c}{\tau}, \quad (2)$$

where  $F$  is the incoming flux and  $\tau$  is the typical adatom desorption time. The kinetic boundary conditions for the concentration in the vicinity of the steps are obtained by an assumption of linear kinetics, i.e. the diffusion mass flux arriving at the step is taken to be proportional to the departure from equilibrium at the step [2]:

$$\begin{aligned} D\mathbf{n} \cdot \nabla c_+ &= v_+(c_+ - c_{\text{eq}}^*) + v_0(c_+ - c_-), \\ -D\mathbf{n} \cdot \nabla c_- &= v_-(c_- - c_{\text{eq}}^*) + v_0(c_- - c_+), \end{aligned} \quad (3)$$

where  $v_{\pm}$  and  $v_0$  are attachment-detachment and transparency kinetic coefficients, the role of which will be discussed later. The local equilibrium concentration  $c_{\text{eq}}^*$  is computed from the Gibbs–Thomson relation,

$$c_{\text{eq}}^* = c_{\text{eq}} \exp(\mu/k_B T), \quad (4)$$

where  $c_{\text{eq}}$  is the reference equilibrium concentration. One has  $\mu = \Omega\tilde{\gamma}\kappa$ , where  $\kappa$  is the step curvature, and  $\tilde{\gamma} = \gamma + \gamma''$  is the step stiffness, with  $\gamma$  the line tension of the step. When the radius of curvature of the step  $1/\kappa$  is much larger than  $\Gamma = \Omega\tilde{\gamma}/k_B T$ , we may linearize Eq. (4), so that:

$$c_{\text{eq}}^* = c_{\text{eq}}(1 + \Gamma\kappa). \quad (5)$$

Additional contributions to  $\mu$  coming for example from interactions between steps will be considered in the next sections.

Eqs. (1), (3) are not the only possible formulation of the boundary conditions. Indeed, linear combinations of the boundary conditions give rise to new formulations, some of which are listed in [3].

The kinetic coefficient  $v_0$  was introduced in [2], and accounts for ‘direct’ exchange between terraces: this phenomena is called step transparency, or step permeability. When steps are perfectly transparent  $v_0 \rightarrow \infty$ , the boundary conditions can be expressed as

$$c_+ = c_- = c_{\text{eq}}(1 + \Gamma\kappa), +\tilde{\beta}\frac{V_n}{\Omega}, \quad (6)$$

where  $\tilde{\beta} = (\nu_+ + \nu_-)^{-1}$ . This boundary condition is used for solidification fronts [4]. Experimental evidence of step transparency has been found from the decay of small mounds on Si(100) [5], and from electromigration induced step bunching on vicinal Si(111) [6,7].

An important consequence of step transparency is that it makes step dynamics non-local on stepped surfaces. Indeed, when  $\nu_0$  is large, atoms may diffuse through many steps before attachment, allowing a coupling between structures that are far apart.

The second important effect related to step kinetics is the so-called step Ehrlich–Schwoebel effect (sESE), which accounts for the asymmetry between the upper and the lower terraces (i.e.  $\nu_+ \neq \nu_-$ ). Typically, attachment-detachment kinetics from the upper terrace is slower ( $\nu_+ > \nu_-$ ). Nevertheless, mass transport in the step region may be quite complex [8], with kink funnelling, exchange mechanisms, etc., and we shall therefore not exclude the possibility of an inverted sESE.

In non-equilibrium situations, this kinetic asymmetry may result in macroscopic mass fluxes along vicinal surfaces. These orientation-dependent mass fluxes are a major source of pattern formation. For example, they lead to mound formation [11] and step meandering [12] during growth at moderate temperatures, to step bunching during sublimation [13], and to various instabilities under oscillatory driving of the surface [14].

### 1.3. Internal step dynamics

#### 1.3.1. Around equilibrium

On Cu(100) surfaces at room temperature, mass transport is dominated by diffusion of atoms along the steps [15]. On lengthscales larger than the distance between kinks, steps then obey Mullins' model for self-diffusion [16]:

$$V_n = -\partial_s(aD_L\partial_s\mu/k_B T), \quad (7)$$

where  $D_L$  is a diffusion constant, and  $a$  is an atomic length.

The diffusion of mobile atoms along the step edge will lead to the diffusion of monolayer islands. A model based on Eq. (7), and augmented with Langevin forces leads to a cluster diffusion constant  $D_c \sim 1/R^3$  [17], where  $R$  is the radius of the island. However, from the observation of small islands on Cu(100) [18], in agreement with Kinetic Monte Carlo Simulations [19,20], one finds that  $D_c \sim R^{-\alpha}$ .  $\alpha$  varies from  $\alpha = 3$  for large islands and high temperatures, to  $\alpha = 1$  for small islands and low temperatures. Similarly low temperature deviations were observed in temporal correlations of the fluctuations of straight steps on Cu(100) vicinal surfaces [15].

We shall first notice that these observed deviations occur at low temperatures where the distance between thermal kinks  $L_k$  is quite large (using the experimental results of [15] on Cu(100), we find  $L_k \sim 10^2$  at room temperature). When the typical distance between thermal kinks is larger than the island size, we do not expect Eq. (7) to be valid, and the timescale for the motion of a mobile atom along the step is essentially limited by the probability of presence of a thermal kink. In this regime, one finds  $D_c \sim 1/R$ . Using Markov chains for the description of atomic motion, this result has been analyzed in details by Combe et al. [20].

A simple continuum phenomenological model which explicitly accounts for the dynamics of a concentration of mobile atoms diffusing along the step from kink to kink was proposed [21]. This model exhibits low temperature deviations in agreement with the above-mentioned observations, and also provides an expression for the diffusion constant:  $D_L = ac_s D_s / (1 + d/L_k)$ , with  $d = a(\exp(E_{ks}/k_B T) - 1)$  where  $E_{ks}$  is the additional energy needed for an atom to go around a kink,  $c_s$  and  $D_s$  are respectively the concentration and the diffusion constant of mobile atoms along the straight parts of the steps. This expression for  $D_L$  was confirmed by Monte Carlo simulations [22]. Nevertheless, such a simple model does not explain the sintering of two-dimensional islands studied by Liu et al. [23], which involves far from equilibrium concave shapes.

Similar deviations from the macroscopic theories were observed when steps exchange atoms with the terraces. The rate of detachment of atoms from 2D clusters, was for example studied in [24]. We shall also mention that similar problems occur in the context of solution growth. For example, Chernov has pointed out the crucial role of kink emitted by corners for polygonized steps during spiral growth [25].

#### 1.3.2. Far from equilibrium

Let us start with the famous contribution of Kardar, Parisi, and Zhang (KPZ) [26], who proposed a simple nonlinear and general equation for the roughening of fronts during growth:

$$\partial_t \zeta = V + \partial_{xx} \zeta + (\partial_x \zeta)^2 + \eta, \quad (8)$$

where  $\zeta$  is the position of the step,  $x$  is the abscissa along the average step orientation,  $V$  is the velocity of a straight front, and  $\eta$  is a white noise. This model, for example, indicates that the r.m.s. roughness of a long enough step obeys:

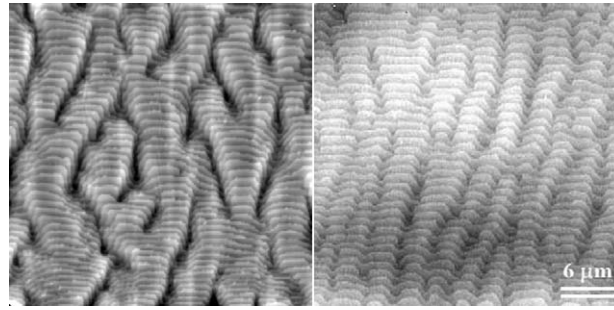


Fig. 2. STM images of step meandering during MBE growth on a vicinal surface. Left panel Cu(1,1,17) surface (Courtesy of L. Douillard, CEA-Saclay, France). Right panel Si(111) vicinal surface at the transition temperature between  $(1 \times 1)$  and  $(7 \times 7)$  (Courtesy of H. Hibino, Atsugi, Kanagawa, Japan).

$W = \langle (\zeta - \langle \zeta \rangle)^2 \rangle^{1/2} \sim t^\beta$ , with  $\beta = 1/3$ . Although there are some numerical checks from Kinetic Monte Carlo simulations [9], we are not aware of experimental evidence in agreement with this model.

Mean field theories have also been developed. For example, it is found in [27] that the kink density along high symmetry steps is proportional to  $V^{1/3}$ . Nevertheless, and once again, we are not aware of an experimental validation of this prediction. Moreover, mean field models do not provide the asymptotic power-law behavior expected from the KPZ model.

An additional complication comes from the presence of reconstructions on the surface. For example, a precise analysis of the kinetics of the GaAs surface [28] seems to show that reconstruction itself may be the origin of complex regimes and morphological instabilities.

In the context of solution growth, mean field models have also been developed. We may for example cite the recent work of Balykov et al. [29], who showed that growth may either lead to roughening or smoothing depending on the precise attachment path of the atoms to the steps.

In many epitaxial systems (such as for Cu(100) surfaces in vacuum already mentioned above), atoms do not detach from the steps, but may diffuse along them. If we assume that no vacancy is created during step motion, the evolution of the step morphology results from a mass flux  $j$  along the step and one has:  $\partial_t \zeta = V + \partial_x j$ . The nonlinear term which occurs in Eq. (8) cannot be written as the divergence of a flux. Hence, other nonlinear terms such as  $\partial_{xx}[(\partial_x \zeta)^2]$  have been included, which in turn lead to new scaling laws for the roughness [30].

In the presence of diffusion along steps, the kink-Ehrlich–Schwoebel effect (kESE), which accounts for the difficulty for atoms to diffuse around a kink, becomes crucial. The kESE has consequences on step stability similar to that of the step Ehrlich–Schwoebel effect (sESE) on the stability of surfaces. For example, Schwoebel [13] has shown that the sESE stabilizes vicinal surfaces during growth. Following the same lines, Aleiner and Suris [31] have shown that vicinal steps are stabilized during growth in presence of kESE. Even more drastic consequences are found for nominal steps, which exhibit a morphological instability similar to Villain’s mounding instability on surfaces [11], leading to the spontaneous formation of step meander during growth [32]. A quantitative study of the shape of the meander [33] reveals that it follows the nonlinear theory developed for sESE-induced mound formation by Politi and Villain [34]. The predictions of this meandering instability seems to be compatible with the observations on Cu vicinal surfaces [35] (see Fig. 2).

A more surprising feature is the formation of mounds in presence of kESE found in [32]. This effect results from an uphill mass flux along vicinal surfaces, which comes from the stabilization of the steps via line diffusion [32]. A detailed analysis of this mass flux indicates that it should also lead to step bunching [36].

#### 1.4. Phase field models

Let us give an explicit example of a phase field model for step motion. The first equation is an evolution equation for the phase field  $\phi$  which is the height of the surface:

$$\tau_p \partial_t \phi = W^2 \nabla^2 \phi - \partial_\phi f + \lambda (c - c_{eq}) \partial_\phi g, \quad (9)$$

where  $W$  is the step width.  $\tau_p$  and  $\lambda$  are constants.  $f$ , and  $g$  are functions of  $\phi$ .  $f$  is an energy density having minima for values of  $\phi$  corresponding to terraces.  $g$  is a coupling function. The second equation accounts for the evolution of the adatom concentration  $c$ :

$$\partial_t c = \nabla[M \nabla c] + F - \frac{c}{\tau} - \partial_t h, \quad (10)$$

where  $M$  and  $h$  are functions of  $\phi$ .  $M$  is the non-constant adatom diffusion constant, and  $h$  is the solid concentration (i.e. the number of solid atoms per unit area above an arbitrary reference level).

The link between phase field models and the discontinuous step model of Section 1.2 is performed via an asymptotic analysis where the width of the interface  $W$  is small as compared to a cut-off length from the diffusion field. In the so-called *sharp interface asymptotics* [37], the coupling constant is small:  $\lambda \sim W$ . In this weak coupling limit, one obtains the strong transparency boundary conditions (6) [3]. Other asymptotics are possible. For example, in the so-called *thin interface asymptotics* [38], one keeps a small deviation from equilibrium at the step, i.e.  $c - c_{\text{eq}} \sim W$ . We therefore obtain a discontinuous step model with fast kinetics [3], where  $v_{\pm} \sim 1/W$ , and  $v_0 \sim 1/W$ . Singular adatom mobility may be used to obtain a significant sESe [39]. In order to obtain arbitrary kinetics, a phase field model with one concentration field per terrace was proposed [3].

Phase field models can for example provide expressions for step kinetic coefficients as a function of the microscopic mobilities [3]. Nevertheless, they have essentially been used up to now as a numerical tool for solving the traditional step model depicted in Section 1.2. Indeed, in the step model, the tracking of the step position on which boundary conditions must be imposed is a delicate and complex task. On the other hand, the determination of the step position and the boundary conditions at the steps are intrinsic properties of the phase field model, which do not have to be computed during the numerical integration. Some examples of use of the phase field models were reported for spiral growth [40], relaxation of bunches [41], growth and nucleation from nominal surfaces [42], step meandering [3], or dynamics of adsorbates with elastic interactions [43]. Statistical fluctuations can also be introduced in phase field models by means of Langevin forces, as shown in [41].

## 2. Step motion

### 2.1. Step meandering

#### 2.1.1. Origin of the meandering instability

Here we shall forget about the complexity of internal steps dynamics, and analyze the motion of steps due to their coupling to adatom diffusion on terraces based on the model of Section 1.2.

In 1990, Bales and Zangwill [12] have showed that the steps are morphologically unstable during growth in presence of a sESe. The instability is due to the fact that the step velocity will be larger in convex step regions due to the geometrical increase of the adatom capture zone when attachment is not symmetric.

The sESe does not have to be localized precisely at the step. Elastic relaxation of the step edges [44] or step induced reconstructions [45] may induce a slower diffusion on the upper terrace in the vicinity of the step leading to the same instability. As shown in Fig. 2, a meandering instability was indeed observed on Si(111) surfaces during growth, where terraces are partially reconstructed in the vicinity of the steps [45].

Another origin of the meandering instability was pointed out in [46] in presence of a drift of the adatoms. Electromigration induced step meandering was observed on Si(111) surfaces at high temperature [47]. Nevertheless, the interpretation of these experiments is still controversial. Other more complex effects may also occur when the electromigration direction is arbitrary [48].

#### 2.1.2. Nonlinear dynamics

The first studies of the nonlinear dynamics of step meander were performed in [49], which focus on the dynamics of the Bales and Zangwill instability in the presence of significant desorption on terraces. The nonlinear dynamical equation is found from a self-consistent expansion of the model equations close to the instability threshold, where the spatio-temporal scales involved in the instability are large. This expansion, called multi-scale analysis, allows one to eliminate the stable short wavelength modes, which relax fast. The meander is then found to obey the Kuramoto–Sivashinsky equation:

$$\partial_t \zeta = -\epsilon \partial_{xx} \zeta - \partial_{xxx} \zeta + (\partial_x \zeta)^2, \quad (11)$$

which leads to spatio-temporal chaos. A full solution of the step model with a phase field approach, as well as kinetic Monte Carlo simulations confirms the existence of the chaotic regime [3,9]. Moreover, when steps are not isolated, i.e. when the distance between steps is smaller than the desorption length on terraces  $x_s = (D\tau)^{1/2}$ , the vicinal surface obeys a two-dimensional anisotropic Kuramoto–Sivashinsky equation, which also leads to chaos [49].

In typical MBE experiments, desorption of adatoms is negligible, and  $\tau \rightarrow \infty$ . The multi-scale analysis reveals features which markedly differ from the previous case. A highly nonlinear evolution equation [50] is obtained for the in phase meander on a vicinal surface:

$$\partial_t \zeta = \partial_x \left[ -\frac{F\ell^2}{2} \frac{\partial_x \zeta}{1 + (\partial_x \zeta)^2} + \frac{\mathcal{M}}{(1 + (\partial_x \zeta)^2)^{1/2}} \partial_x \mu \right], \quad (12)$$

where  $\mathcal{M} = (D\Omega c_{\text{eq}}\ell/(1 + (\partial_x \zeta)^2)^{1/2} + D_L a)/k_B T$ , and  $\ell$  is the interstep distance. As will be discussed in Section 3, interactions of elastic origin are present between steps. This leads to an additional term in the chemical potential [51]:

$$\mu = \Omega \kappa \left( \tilde{\gamma} + \frac{3A}{\ell^2} (1 + (\partial_x \zeta)^2)(1 + 2(\partial_x \zeta)^2) \right), \quad (13)$$

where  $A$  is the elastic interaction constant. The step stiffness is therefore corrected with a nonlinear contribution coming from elastic interactions.

Eq. (12) leads to meandering ripples whose amplitude grows in time as  $t^{1/2}$ . In absence of elastic interactions, the lateral wavelength is fixed from the first stages of the instability. Nevertheless, endless coarsening of the meandering ripples is obtained when  $A \neq 0$ . The amplitude and coarsening exponents can be calculated from a heuristic self-affine ansatz, as shown in [51].

In presence of anisotropy, Danker et al. [52] have shown that a different scenario appears, where the wavelength of the meander freezes after some finite amount of coarsening. Asymptotically, the amplitude of the meander still increases as  $t^{1/2}$ . This scenario leads to a nonlinear wavelength selection mechanism. Unexpectedly, the final wavelength may also be selected by a pre-patterning of the substrate [52].

These results on meandering exhibit some generic features of the nonlinear dynamics of non-equilibrium fronts. Indeed, when an instability occurs in the vicinity of thermodynamic equilibrium in a conserved system, the dynamics is always highly nonlinear [53]. Moreover, the existence of only three possible scenarios (no coarsening, interrupted coarsening or endless coarsening) is related to the structure of the steady-states, as shown in [54].

## 2.2. Step bunching

### 2.2.1. Mechanism of the instability

Another instability is the formation of bunches of steps from a vicinal surface (Fig. 3). Step bunching may be caused by a wide variety of effects, such as an ES effect during sublimation [13], the presence of impurities [55], elastic relaxation of step edges [44], or electromigration [56]. Therefore, following [57], we shall consider a simple model where the velocity of a step is a function of the width of the neighboring terraces only:

$$V = f_+(\ell_+) + f_-(\ell_-). \quad (14)$$

We now want to analyze the stability of a vicinal surface where step velocities obey equation (14). If the average distance between the steps is  $\ell$ , the average step velocity is  $V = f_+(\ell) + f_-(\ell)$ . We then consider a small perturbation  $\zeta = \exp(\omega t + i n \phi)$  of the position of the steps, so that the position of the  $n$ th step is  $n\ell + \zeta_n$ . From the linearization of Eq. (14), we find:

$$\omega = (1 - \cos(\phi))\partial_\ell \Psi + i \sin(\phi)\partial_\ell V, \quad (15)$$

where  $\Psi = f_-(\ell) - f_+(\ell)$ . The perturbations are unstable if the real part of  $\omega$  is positive, i.e.  $\partial_\ell \Psi > 0$ ; they are stable when  $\partial_\ell \Psi < 0$ . Hence, the origin of the instability is a bias towards the upper terrace of the sensitiveness of the step velocity to the width of the neighboring terraces [57], which can be written:  $\partial_\ell f_-(\ell) > \partial_\ell f_+(\ell)$ . At long wavelengths,  $\Psi$  is the mass flux along the surface, and the stability criterion can be related to the variations of  $\Psi$  as a function of the step density [58]. Nevertheless, we shall not adopt this language here, which is not adapted to the description of non-continuous step densities, or pairing instabilities mentioned below.

We shall also mention that step bunching is not always a kinetic instability, i.e. bunches are sometimes observed in absence of a linear instability. Bunching can then be understood as the production of shock waves within kinematic wave theory [59]. Such a situation may be found during etching [60].

### 2.2.2. Nonlinear dynamics

A multiscale analysis of the kinetic instability can be performed following the same lines as in Section 2.1.2. The resulting equation is the Benney equation:

$$\partial_t \zeta = -\epsilon \partial_{yy} \zeta - b \partial_{yyy} \zeta - \partial_{yyyy} \zeta + (\partial_y \zeta)^2, \quad (16)$$

where the surface height  $y$  is obtained from the continuum limit of the step indexes. When the parameter  $b$  is large enough, the dynamics lead to an array of ordered bunches. When  $b$  is small, one recovers the spatio-temporal chaos related to the KS limit equation (11). In the case of electromigration-induced step bunching [61],  $b$  is large, and the ordered regime is observed. The Benney equation was also found for the meandering of anisotropic steps [62].

As in the case of step meandering, when desorption is small, the multi-scale analysis shows that bunching dynamics may be highly nonlinear.<sup>1</sup> The evolution equation for the surface profile is now [64]:

<sup>1</sup> This is not a general rule, and a weakly nonlinear equation can be obtained, such as in [63].

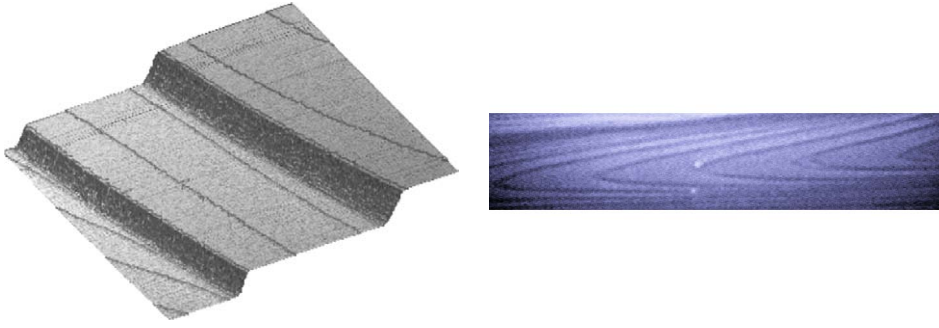


Fig. 3. Left panel: STM image step bunching on Si(111) under electromigration (Courtesy of E.D. Williams). Right panel: Reflection Electron Microscopy image of kinetic pairing of identical steps on Si(111) under electromigration.

$$\partial_t \zeta = a D c_{\text{eq}}^0 \partial_y \left[ \frac{1/\xi - a A \rho \partial_{yy} \rho^3}{1 + d\rho} \right], \quad (17)$$

where  $\rho = 1/(\ell - a\partial_y \zeta)$  is the local step density. The numerical solution of Eq. (17) shows that the amplitude of the perturbation increases rapidly and the step density approaches zero at some singular points [64]. At these points, wide terraces appear, and bunches become separate entities. The separation of the bunches is observed in most step bunching experiments. Once bunches are separated, the continuum approach breaks down. Therefore, the coarsening exponents can be extracted from a detailed analysis of the morphology of the bunches, as done in [66,57,64,67]. Another approach has been suggested for step bunching during growth [65], following the same power-counting method as in [51]. Nevertheless, the role of the singularities of the density profile on the coarsening dynamics is not yet understood.

### 2.3. Step pairing

An instability towards a stable train of pairs was recently observed on Si(111) surfaces under electromigration around 1230 °C [7]. Using a step model, it was shown that this instability is a non-local effect, which can be obtained when steps are very transparent. Surprisingly, the experimental observation of this instability indicates that the transparency kinetic coefficient  $v_0$  in Eq. (3) is negative. With the help of a phase field model [3], this can be traced back to a faster adatom diffusion in the step region.

A qualitatively different scenario is observed on Si(100) during growth[68]. Indeed, the surface then exhibits an alternated dimer-row reconstruction  $(1 \times 2)/(2 \times 1)$  from one terrace to the other. Therefore, there are two types of steps denoted  $S_A$  and  $S_B$ . Since the attachment kinetics is different on  $S_A$  and  $S_B$  steps, these move at different velocities and kinetic pairing is observed during growth. The faster steps are the  $S_B$  steps, which are rougher and exhibit more attachment sites than  $S_A$  steps. This train of pairs of steps is then unstable with respect to step bunching [68]. In Section 3, we will see that there is also a step pairing transition of energetic origin on these surfaces.

### 2.4. Monolayer islands

#### 2.4.1. Growth

During the growth of monolayer islands at low temperatures, atoms which are attached to a step cannot move to a neighboring site of lower energy. This conditions correspond to the regime of Diffusion Limited Aggregation (DLA), and the resulting island shape is fractal. At higher temperatures, local relaxation at the steps is possible. Nevertheless, the steps may be unstable because of: (i) internal steps dynamics, such as that related to line diffusion with a kESE; (ii) an asymmetric coupling to the diffusion field, as mentioned in Section 2.1.2, coming from the sESE [69], or from the asymmetry of the terrace widths adjacent to a step. This latter meandering scenario was observed by Homma et al. [70].

#### 2.4.2. Migration

When mobile atoms drift (e.g. in presence of electromigration), two-dimensional islands may also drift. The occurrence and direction of the drift depend on the dominant mass transport mechanism and on the presence of a sESE [10]. This drift was observed for monolayer islands on Si(100) and Si(111) [71]. The latter case leads to the first proof of the presence of an sESE on Si(111).

The morphological stability of islands under electromigration was studied in [10]. Depending on the mass transport mechanism, island splitting or slit formation was found.

### 3. Elastic relaxation

Adding a defect (e.g. a step, an atom, a reconstruction phase boundary) at the surface of a crystal leads to an additional localized distribution of forces around the defect, which has two main consequences: (i) firstly, this leads to an interaction energy between two defects; and (ii) secondly, the displacement field induced by a defect will change the diffusion barriers of the mobile atoms. Therefore, kinetics will also be affected by the elastic relaxation of the crystal.

#### 3.1. Interaction between defects

From mechanical equilibrium, the leading order contribution of the forces around a punctual defect is a dipole. The elastic interaction energy between two defects separated by the distance  $r$  is therefore found to be repulsive and  $\sim 1/r^3$  [72]. Peyla and Misbah [73] have shown that anisotropy may drastically change this picture, changing the sign, or the power law exponent for these interactions.

If a linear defect at the surface separates two identical surfaces, a density of dipoles is located in its vicinity, which leads to an interaction energy between parallel linear defects  $\sim 1/r^2$  [74]. Nevertheless, if the linear defect separates two surfaces which exhibits different surface stress tensors, mechanical equilibrium now imposes the presence of a density of forces along the defect. The interaction energy per unit length is then  $\sim \ln(r)$ . These interaction energies are of course modified in presence of step meander [75].

Such logarithmic interactions are found on Si(100) surfaces, which exhibits a bi-periodic ( $1 \times 2$ ) reconstruction, turned from 90 degrees from one layer to the next one. These two types of steps have the possibility to form double steps of lower energy. Nevertheless, the strong logarithmic interaction of single steps allows the surface to gain an energy proportional to the logarithm of the terrace width. Therefore, single steps are stabilized for small miscut angles [76].

In the case of hetero-epitaxy, the lattice mismatch between adsorbate and substrate leads to a stress accumulation in the adsorbate. A step on the adsorbate surface may therefore also be seen as a linear defect separating two different surfaces, the accumulated stress being larger on the higher side.

Feng Liu et al. [77] have shown that during hetero-epitaxy, a train of steps can be destabilized by the logarithmic attractive interactions between steps. Combining growth and the destabilizing effect of the elastic interactions, arrays of bunches with long range order may be obtained.

A phononic contribution to the interaction energy between surface defects is also present, which is not always negligible [78].

#### 3.2. Kinetics

Elastic relaxation may also affect adatom diffusion, and doing so, it may also produce kinetic asymmetries which are a source of morphological instabilities. As an example, Duport, Nozières and Villain [44] have shown that elastic relaxation in the vicinity of the step edges may lead to a change of the mobility of adatoms thereby leading to an effective ES effect, or inverted ES effect. Therefore, step bunching or step meandering could be observed. This effects may also change significantly the dynamics of submonolayer growth, as mentioned by Wolf et al. [79].

The Stransky–Krastanov growth mode, where 3D growth is preceded by growth of some complete mono-layers, will be discussed in details in another contribution of the present issue. We shall therefore only briefly mention how step motion comes into play in the early stages of this growth mode.

First, it was shown, for example in [80], that the initial stages of growth in Si/Ge at low misfits exhibit a large kinetic roughness of the surface. One can therefore conclude that a continuum model for the surface is more adapted than a step model. Nevertheless, designing a continuum model which quantitatively accounts for the kinetic roughness is a delicate matter [81]. In the case of high misfits, the role of steps as possible nucleation sites was recently suggested by Villain [82].

In the next stage of this growth mode, Molecular Dynamics studies [83] and experiments of Ag/Si [84] indicate that matter is sometimes sucked from the wetting layer to form 3D mounds. This dewetting process seems to be controlled by the dynamics of individual steps.

### 4. Electronic relaxation

Electronic relaxation leads to effects that are similar to that of elasticity, i.e. interactions between defects [85] and should also change the kinetics. The novelty here is the possibility of oscillatory interactions.

For example, the interaction between defects on metal surfaces result from the screening of the perturbation by conduction electrons. The interaction energy between adatoms is  $\sim \cos(2k_F r)/r^m$ , and between steps  $\sim \cos(2k_F r + \pi/4)/r^{m-1/2}$ . One



finds that  $m = 5$  when the interaction is mediated by the bulk electronic surface states, but  $m = 2$  when the interaction is mediated by surface states [85]. The oscillatory character of the interactions was confirmed by experiments [86,87].

In thin metallic layers, the total electronic contribution to the energy results from a delicate interplay between quantum confinement of the electrons, charge spilling in the substrate, and interface induced Friedel oscillations. The stability of metallic adsorbates was found to be affected by these effects by Zhang et al. [88]. One of the most striking effects is the existence of magic thicknesses, which were observed in experiments for the growth of Ag/GaAs [89].

## 5. Conclusion

We have presented a rapid overview on recent advances and open questions about step dynamics on crystal surfaces. This brief review has of course missed many topics in the very active research field of step dynamics, and the reader is invited to consult extended reviews [90,91,25,30,34].

We would also like to mention the recent progress on the persistence of step fluctuations [92]. The competition between statistical noise and deterministic chaotic meander was also a great achievement for the roughening theories [93]. Moreover, studies on irreversible nucleation [94] and on mound formation [34], have now reached a mature level of understanding.

To conclude, the past 15 years have seen a drastic improvement of the understanding of step dynamics. These advances will provide tools for a better control of the morphology of nanostructures.

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