Ripples and ripples: from sandy deserts to ion-sputtered surfaces

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Abstract. We study the morphological evolution of surfaces during ion sputtering and we compare their dynamical corrugation with aeolian ripple formation in sandy deserts. We show that, although the two phenomena are physically different, they must obey similar geometrical constraints and therefore they can be described within the same theoretical framework. The present theory distinguishes between atoms that stay bounded in the bulk and others that are mobile on the surface. We describe the excavation mechanisms, the adsorption and the surface mobility by means of a continuous equation derived from the study of dune formation on sand. We explore the spontaneous development of ordered nanostructures and explain the different dynamical behaviours experimentally observed in metals or in semiconductors or in amorphous systems. We also show that this novel approach can describe the occurrence of rotation in the ripple direction and the formation of other kinds of self-organized patterns induced by changes in the sputtering incidence angle.
1. Introduction

When an ion hits a surface, it liberates locally a large amount of energy that generates cascades of collisions in the bulk inducing an effective instantaneous melting of a region of the solid immediately below. For geometrical reasons, the effect of ion bombardment depends on the surface curvature: the energy concentrates on regions of positive curvature and this favours the excavation of valleys and the growth of hills [1, 2]. On the other hand, thermal diffusion and surface tension tend to smoothen the irregularities by reducing roughness and flattening the surface. It has been observed that under the combined action of these mechanisms, the surface tends to spontaneously create ripples [3]–[14]. In nature, ripples are commonly observed in sandy deserts as the result of dynamical instability of the sand surface under the action of a sufficiently strong wind [15]. In this case, the formation of ripples is commonly associated with the effect produced by some grains that are lifted from the sand bed and accelerated by the wind. These grains, re-impacting with the bed splashing up a number of other grains. Most of these grains return to the bed leading to a local rearrangement, whereas some others are accelerated by the wind.
and impact again after a certain ‘saltation’ length. In the literature, many studies have been devoted to understanding the mechanism of ripple formation [16]–[21]. In particular, a hydrodynamical model for aeolian ripple formation, based on a continuum dynamical description with two species of grains (immobile and rolling grains), was proposed successfully by Bouchaud et al [22]–[27]. The main ingredient of such a model is a bilinear differential equation, for the population of the two species of grains, which leads to the instability of a flat bed against ripple formation.

In this paper, we show that the same reasoning which has been used to describe the sand ripple formation in deserts, when applied to the studies of dynamical surface roughening, leads to an accurate description of the morphogenesis and evolution of ripples on crystal and amorphous surfaces during ion sputtering (see figure 1). The present approach contains, and extends, the Bradley–Harper approach [28] and its nonlinear extension by Rost and Krug [29] and by Park et al [30] (based on a Kuramoto–Sivashinsky and Kardar–Parisi–Zhang type equations [31, 32]). The approach presented here describes some of the crucial experimental features observed in these systems [9]. In particular, we can describe the two distinct dynamical behaviours experimentally observed in amorphous or semiconductor systems and in metals [7]. In the first case (amorphous/semiconductors), we find that the ripples grow exponentially fast at constant wavelength \( \sim \hat{l} \), up to a critical roughness (the root mean square of the height profile [33]) \( W_c \) at which the growing process interrupts. On the other hand, in metals (when the Erlich–Schwoebel barrier is active), we can observe a transition between an initial exponential to a slower growth of the root mean square of the height profile. In this regime the ripple wavelength is also growing with time and re-nucleation effects are observed. We show that, self-organized nanostructures can develop spontaneously on a surface under ion bombardment producing ripples, dots and other organized patterns and we demonstrate that the intriguing phenomenon of ‘ripple-rotation’ [9], associated with a change in the sputtering incidence angle, can be described.

The main novelty of this work is the use of a new kind of equation to describe the surface instabilities under ion bombardment. In the present approach we clearly distinguish between three mechanisms: (i) erosion; (ii) adsorption–condensation; and (iii) mobility. Physically, all
these three mechanisms take place simultaneously at a surface under ion bombardment. The possibility to distinguishing between them clarifies the approach, simplifies the choice of the parameters and enlarges the descriptive power of the theory. Moreover, we distinguish between atoms that stay in the bulk in bounded position and others that stay on the surface and are mobile. This (simplified) view is more realistic than considering the whole system as a fluid. We note that these novel elements of the present theory do not introduce, per se, extra parameters in the analogy with the well-established Bradley–Harper theory [28]. However, our choice in this paper has been to study the equations in their most complete form, thus introducing extra parameters.

This paper is organized as follows. In section 2, the differential equation describing both sand ripples and surface corrugation under ion bombardment is introduced and discussed. In sections 3 and 4, the dispersion relation is obtained by means of a linear stability analysis. The initial wavelength of the fastest growing modes is calculated by using a standard approximation (section 5) and, in some special cases, by finding exact solutions (section 6). Results from numerical solutions are reported in section 7. Section 8 summarizes the main results and perspectives.

2. Particle mobility and ripple dynamics

When the surface of a solid is taken under ion bombardment some atoms in the proximity of the surface receive energy from the ions and pass from a bounded, ‘immobile’, solid state to a ‘mobile’ melted state. The opposite mechanism also takes place: some mobile atoms can find a lower energetical state by becoming immobile and bounding in a given position. Other atoms, or clusters of atoms, can break the bonds and be sputtered away from the surface; a part of them will be redeposited, whereas a fraction might be dispersed.

In analogy with the theory developed to explain the dynamical evolutions of dunes in deserts [22]–[25], we describe the mechanisms of excavation, exchange between mobile and immobile atoms and surface displacement of mobile atoms in terms of the following differential equation:

\[
\frac{\partial h}{\partial t} = - \Gamma(R, h)_{ex} + \Gamma(R, h)_{ad}
\]

\[
\frac{\partial R}{\partial t} = - \nabla J(R, h) + (1 - \phi) \Gamma(R, h)_{ex} - \Gamma(R, h)_{ad},
\]

where \( h(r, t) \) is the height of surface profile made of immobile-bounded atoms and \( R(r, t) \) is the height of mobile-melted atoms. In equation (1), \( \Gamma(R, h)_{ex} \) and \( \Gamma(R, h)_{ad} \) are respectively the rates of atoms that are excavated (ex) and adsorbed (ad) under the action of the sputtering, \( (1 - \phi) \) is the part of excavated atoms that pass from immobile to mobile, and \( \phi \) is the fraction that does not redeposit on the surface, whereas \( J(R, h) \) is the current of mobile atoms which displace on the surface. (In this paper, we label positions and directions on the surface in terms of a cartesian system of coordinates \((x, y)\).)

Let us now examine and explain in detail the various terms contained in equation (1).

2.1. Excavation

The excavation effect must depend on the number and velocity of the sputtered ions (i.e. its flux), but also the local shape and orientation of the surface might play an important role. Indeed,
the energy transmitted by the impacting ions concentrates more in regions of the surface with positive curvature. Moreover, part of the surface facing the flux is likely to experience a different erosion with respect to others that are less exposed to the flux. In the literature, such dependence of the sputtering yields on the surface curvature and on the incoming ion-flux orientation has been described in great detail (see for instance [7] and references therein). Here, we adopt the same reasoning that led to the Bradley and Harper equation [28] and we take into account possible anisotropies and crystalline orientations (metals). We write

$$\Gamma(R, h)_{ex} = \eta \left[ 1 + a \nabla h + \left( b_x \frac{\partial^2}{\partial x^2} + b_y \frac{\partial^2}{\partial y^2} \right) h \right].$$ (2)

Here $\eta$ is the sputtering flux; $a = (a_x, a_y)$ is a vectorial parameter associated with the flux direction-dependent erosion, and $b_x, b_y$ are associated with the curvature-dependent sputtering erosion (i.e. erosion is more efficient at surface depressions). All these terms are implicitly dependent on the orientation of the incoming ion flux, this in analogy with [28]. (For instance, for oblique incidence: $|a|, b_x, b_y \propto \sin \theta$, with $\theta$ the angle between the direction of the ion beam and the normal to the surface.)

A noise term $\epsilon(x, y, t)$ can be eventually added to equation (2). This term mimics the fact that the incoming flux is made of discrete particles and in experiments certain amounts of noise and randomness are unavoidable.

2.2. Adsorption

The rate of adsorption of mobile atoms into the solid bulk must depend on the quantity of mobile atoms at a given spatial position. Similarly to the excavation process, the adsorption is also dependent on the local curvature and orientation. We can write

$$\Gamma(R, h)_{ad} = R \left( \gamma + c \nabla h + \left( d_x \frac{\partial^2}{\partial x^2} + d_y \frac{\partial^2}{\partial y^2} \right) h \right).$$ (3)

where the parameter $\gamma$ is the recombination rate and $c = (c_x, c_y)$ and $(d_x, d_y)$ are associated to the different probabilities of recombination in relation with the local orientation and shape of the surface.

Note that equations (2) and (3) contain the same terms as the ones proposed in the literature for the formation of aeolian dunes in the so-called hydrodynamical model [22]–[25, 34]. Indeed, in deserts, sand grains are lifted from the sand bed and readsorbed into it with a probability which is dependent on the local shape and orientation of the dunes. Equations (2) and (3) represent the simplest analytical expressions which formally take into account these shape and orientation dependences. In the quest for simple explanations, such equations are therefore rather universal.

2.3. Mobility

Mobile atoms displace on the surface, and the quantity $J(R, h)$ in equation (1) is their ‘current’. In surface growth, there are two main mechanisms that are commonly indicated as responsible

3 In the case of aeolian ripples the curvature-dependent terms $b_x, b_y, d_x$ and $d_y$ are isotropic (equal in the $x, y$ directions) and the second derivatives in equations (2) and (3) become proper Laplacians.
for the surface mobility of atoms [35]. The first is a current, driven by the variations of the local chemical potential, which tends to smoothen the surface asperity moving atoms from hills to valleys. The second is a current induced by the Erlich–Schwoebel barrier (metals only) which, in contrast, moves atoms uphill. In addition to these main mechanisms, we might also have to take into account a drift velocity and a random thermal diffusion, obtaining

\[
\mathbf{J}(R, h) = K R \nabla (\nabla^2 h) + s R \frac{\nabla h}{1 + (\alpha_d \nabla h)^2} + v R - D \nabla R.
\] (4)

In this equation, the first term describes a deterministic diffusion driven by the variations of the chemical potential which depends on the local shape of the surface; the second term is associated with the uphill current due to the Erlich–Schwoebel barrier and \(\alpha_d\) is a parameter associated with the characteristic length. The quantity \(\mathbf{v} = (v_x, v_y)\) is a drift velocity of the mobile atoms on the surface which can be associated to the fact that atoms sputtered by an off-normal ion flux tend to be re-adsorbed in a position which is shifted from the excavation point. The parameter \(D\) is instead the dispersion coefficient associated with the random thermal motion. This term is related with a non-deterministic diffusion mechanism and it could mimic the evaporation–condensation effects.

Note that equation (4) is substantially different from the one proposed in the literature to describe ripples in granular media [22]–[24, 33, 36]. Here, the current depends on the local shape and orientation of the surface (the \(h(r, t)\) profile). The equations describing sandy deserts can be retrieved from equation (4) by imposing \(K = 0\) and \(s = 0\), but, in contrast, in surface growth these two parameters are the leading terms of the equation and play the role of control parameters in the dynamics of ripple formation. Nonetheless, these terms describe a rather simple dependence of the dynamics on the geometrical shape of the surface. We expect that similar terms can be profitably introduced in the context of aeolian sand ripples in order to describe specific phenomena (associated, for instance, with packing properties [37] or granular flow [38]) which relate the dynamics of grains with the dune shapes.

It should be noted that the factors \(a, c\) and \(v\) in equations (2)–(4) are vectors (i.e. they have two distinct components in the Cartesian \((x, y)\) directions). Indeed, in general, crystal surfaces are anisotropic and a certain degree of anisotropy can be induced in amorphous system by off-normal sputtering. Therefore, one must take into account the dependence of the parameters on the relative orientation of both the ion bombardment direction and the crystal surface (metals). In equation (4) the parameter \(K\) is assumed isotropic. On the other hand, on crystalline surfaces, anisotropic deterministic diffusions along different crystalline directions are expected and sometimes might play an important role [30]. The extension of the results presented in this paper to the case of anisotropic \(K\) is straightforward.

3. Dispersion relation

A trivial solution of equation (1) is a flat surface which is eroded with a rate \(\phi\eta\): \(h(r, t) = h_0(t)\) and \(R(r, t) = R_0\) with \(R_0 = (1 - \phi)\eta/\gamma\) and \(h_0(t) = -\phi\eta t + \text{const.}\) But this solution is only hypothetical since, in general, the dynamics of the surface profile presents instabilities against spontaneous roughening and therefore its evolution is more complex. Numerical solutions of equation (1) show that periodic ripples or other self-organized patterns can form spontaneously.
Numerical solutions of equation (1) at various times indicate that under the action of ion sputtering the surface develops an instability which leads to the formation of periodic ripples with a well-defined characteristic wavelength. In the figure, the black line is the final surface profile, whereas the thinner green lines are some profiles at previous times. See appendix D for details. The simulation time is in arbitrary units. Typically, we run between $10^3$ and $10^6$ time steps, depending on the system parameters.

![Figure 2](image)

**Figure 2.** Numerical solutions of equation (1) at various times indicate that under the action of ion sputtering the surface develops an instability which leads to the formation of periodic ripples with a well-defined characteristic wavelength. In the figure, the black line is the final surface profile, whereas the thinner green lines are some profiles at previous times. See appendix D for details. The simulation time is in arbitrary units. Typically, we run between $10^3$ and $10^6$ time steps, depending on the system parameters.

A numerical solution of equation (1) in two dimensions. See appendix D for details.

![Figure 3](image)

**Figure 3.** A numerical solution of equation (1) in two dimensions. See appendix D for details.

Some numerical results are shown in figure 2 (for the one-dimensional case) and in figures 3 and 7–9 (for the two-dimensional case).

### 3.1. Stability

In order to infer indications about the amplification or the smoothing of small perturbations and to deduce an analytical expression for the ripples’ wavelength at their beginning, we perform a stability analysis on equation (1). Conveniently, we can assume that the surface profile is made by the combination of a flat term plus an undulated part:

$$ R(r, t) = R_0 + R_1(r, t), \quad h(r, t) = h_0(t) + h_1(r, t) $$

with $R_1(r, t) = \hat{R}_1 \exp(i\omega t + ikr)$ and $h_1(r, t) = \hat{h}_1 \exp(i\omega t + ikr)$. We can then substitute these quantities into equation (1) and linearize the equation by taking only the first order in $R_1$ and $h_1$. 

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A Fourier analysis (see appendix A) shows that such a linearized equation admits solutions when the frequencies $\omega$ and the wave vectors $k$ satisfy:

\[
[i\omega + \gamma + i k v + k^2 \mathcal{D}] [i \omega + i k (v_1 - (1 - \phi) v_2) - k^2 (D_1 - (1 - \phi) D_2)]
\]

\[ - \gamma (1 - \phi) [i k (v_1 - v_2) - k^2 (D_1 - D_2 - s_1) - k^4 K_1] = 0,
\]

where, in order to simplify the equations, we have introduced the following notation:

\[
v_1 = \eta a, \quad v_2 = \eta c / \gamma, \quad s_1 = \eta s / \gamma, \quad K_1 = \eta K / \gamma
\]

\[
\mathcal{D}_1 = \eta (b_x \cos(\alpha)^2 + b_y \sin(\alpha)^2), \quad \mathcal{D}_2 = \eta \gamma (d_x \cos(\alpha)^2 + d_y \sin(\alpha)^2)
\]

where $\alpha$ is the azimuthal angle corresponding to a given direction of $k$ in the $(x, y)$ plane (therefore $k_x = |k| \cos(\alpha), k_y = |k| \sin(\alpha)$). Equation (6) establishes a dispersion relation $\omega(k)$ that is a complex function with two branches corresponding to the solutions of the quadratic equation (6).

Note that this dispersion relation (equation (6)) can be transformed into the corresponding equation in the Bradley–Harper theory [28] when the coefficients $\mathcal{D}, v, s, a, \gamma, c, d, s, K_1, D_2$ and $v_2$ are set equal to zero.

4. Surface instabilities

The kinetic growth of the surface instability is related to the imaginary part of $\omega(k)$. Indeed, $\text{Im}(\omega(k))$ corresponds to modes with amplitudes that change exponentially fast in time, and negative values correspond to unstable modes that increase with the time. We can therefore study $\text{Im}(\omega)$ from the solution of equation (6) and search for the region of $k$ in which $\text{Im}(\omega)$ is negative. The most unstable mode is the one that grows faster and it corresponds to the value of $k$ at which $\text{Im}(\omega)$ reaches its most negative value (see figures 4, 5 and B.1).

The solution of equation (6) for $\text{Im}(\omega)$, is

\[
2 \text{Im}(\omega)_+ = \gamma + [\mathcal{D} - \mathcal{D}_1 + (1 - \phi) \mathcal{D}_2] k^2 \pm \sqrt{\Delta_1 + (\Delta_1^2 + 4 \Delta_2^2)^{1/2}},
\]

where

\[
\Delta_1 = \gamma^2 - [(v - v_1 + (1 - \phi)v_2) k]^2 + 2 \gamma [\mathcal{D} - (1 - 2\phi) \mathcal{D}_1 + (1 - \phi) \mathcal{D}_2 + 2(1 - \phi) s_1] k^2
\]

\[ + [[(\mathcal{D} + \mathcal{D}_1 - (1 - \phi) \mathcal{D}_2) - 4 \gamma (1 - \phi) K_1] k^4
\]

and

\[
\Delta_2 = \gamma [v + (1 - 2\phi)v_1 - (1 - \phi)v_2] k + [\mathcal{D} + \mathcal{D}_1 - (1 - \phi) \mathcal{D}_2][v - v_1 + (1 - \phi)v_2] k^3.
\]

Let us first observe that at zero ion flux (i.e. when $\eta = 0$ and therefore, $v_1 = 0, v_2 = 0, \mathcal{D}_1 = 0, \mathcal{D}_2 = 0, s_1 = 0, K_1 = 0$) the solutions of equation (6) are $\omega(k) = 0$ and $\omega(k) = -k v + i(\gamma + k^2 D)$. In this case, the imaginary part of $\omega(k)$ is non-negative, therefore we expect
Figure 4. The imaginary part of the dispersion relation $\text{Im}(\omega)$ can assume negative values which are associated with the surface instability (arbitrary units). The amplitude of modes with wavelengths $\lambda > 2\pi/k^*$ will grow exponentially fast. The thick line is the imaginary part of the analytical solution of equation (6), whereas the thinner grey line is the approximated expression (at the fourth order in $k$) obtained for small-ion flux ($\eta$ small). (In this figure the parameters are: $\gamma = 8$, $\phi = 0.5$, $\nu = 0.4$, $D = 0.2$, $K_1 = 0.06$, $s_1 = 0.09$, $v_1 = 0.01$, $v_2 = 0.001$, $D_1 = 0.015$ and $D_2 = 0.023$.)

no spontaneous corrugation of the surface (as it must be in absence of ion bombardment). On the contrary, when the sputtering is active ($\eta > 0$), the imaginary part of $\omega(k)$ can assume negative values. This is shown in figure 4 where a plot of $\text{Im}(\omega)$—as a function of $k$ is reported (along a given direction of the vector $k$). As one can see in figure 4, the branch $\text{Im}(\omega)$—takes negative values for $|k|$ between 0 and a critical value $k^*$ at which it crosses the zero. The analogue two-dimensional plots are given in figures 5 and B.1. Other cases are shown in figure B.2 and discussed in appendix B. The critical point $k^*$ (a contour in two-dimensions, see figures 5 and B.1) fixes the minimal unstable wavelength. We therefore expect to find unstable solutions associated with the formation and evolution of ripples with wavelengths $\lambda \geq \lambda^* = 2\pi/k^*$.

5. Wavelength of the fastest modes

Several analytical solutions of equation (6) can be found in some special cases which are discussed in section 6. But the study of the surface instabilities can be highly simplified if we consider the first-order effects when the sputtering flux $\eta$ is small.

5.1. Approximate equation

In the case of small-ion flux, the branch of $\text{Im}(\omega(k))$, with negative values can be approximated to

$$\text{Im}(\omega) \simeq \frac{P_1 k^6 + P_2 k^4 + P_3(k) k^2 + P_4(k)}{D^2 k^4 + 2\gamma D k^2 + (\nu k)^2 + \gamma^2}.$$
Figure 5. Surface plot and contour-line plot for the imaginary part of the dispersion relation Im(ω) from the analytical solution of equation (6) in the two-dimensional case. The plots on the left side have parameters: \(v, v_1, v_2\) and \(s = 0, \gamma = 0.05, \eta = 1, D = 0.1, b_x = 0.25, b_y = 0.5, d_s = 0.025, d_y = 0.025, K_1 = 0.833, \phi = 0.2\). The right plots use the same set of parameters with \(b_x\) and \(b_y\) exchanged.

With

\[
P_1 = D[(1 - \phi) \gamma K_1 - D(D_1 - (1 - \phi)D_2)],
\]
\[
P_2 = (1 - \phi) \gamma [D(D_2 - s_1) + \gamma K_1] - (1 + \phi) \gamma DD_1,
\]
\[
P_3(k) = -[D_1 + (1 - \phi)D_2]\left(\text{vk}\right)^2, \quad P_4 = \gamma^2[(1 - \phi)s_1 - \phi D_1],
\]
\[
P_5(k) = (1 - \phi)\gamma(\text{vk})(v_1 - v_2)k. \quad (11)
\]

When \(k = |k|\) is sufficiently small \((k \ll \gamma/\eta)\), we can develop equation (10) at the fourth order and obtain

\[
\text{Im}(\omega) \approx Ak^4 - Bk^2, \quad (12)
\]

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with

\[
A = (1 - \phi) \left[ K_1 + (s_1 + D_2 - D_1) \frac{y^2 + v^2}{y^2} + v(v_1 - v_2) \frac{2y^2 + v^2}{y^3} \right],
\]

\[
B = \phi D_1 + (1 - \phi) \left[ s_1 + \frac{v(v_1 - v_2)}{y^2} \right].
\]

(13)

Here, \(v, v_1\) and \(v_2\) are respectively the components of \(v\), \(v_1\) and \(v_2\) in the direction parallel to \(k\) (i.e. they are: \(v = |v| \cos(\hat{\mathbf{k}})\); \(v_1 = |v_1| \cos(\hat{\mathbf{v}_1} \mathbf{k})\) and \(v_2 = |v_2| \cos(\hat{\mathbf{v}_2} \mathbf{k})\)).

A comparison between this approximate solution and the exact solution is given in figure 4. Note that this approximate expression admits a negative minimum only if the two terms \(A\) and \(B\) are both larger than zero. Otherwise, for \(A > 0\) and \(B < 0\) the negative minimum disappears, whereas for \(A < 0\) the instability moves at \(|k| \to \infty\) (see appendix B for a discussion of the exact case).

5.2. Solutions

The expected wavelength of the ripples is associated with the fastest growing mode, which corresponds to the value of \(k\) at which \(\text{Im}(\omega)\) reaches its most negative point. From equation (12), the minimum of \(\text{Im}(\omega)\) is at

\[
\hat{k} = \sqrt{\frac{B}{2A}}.
\]

(14)

Therefore, at the beginning, the ripples’ amplitude will grow exponentially fast as \(W \sim \exp(B^2t/4A)\) with associated ripple wavelength at

\[
\hat{\lambda} \sim 2\pi \sqrt{\frac{2A}{B}}.
\]

(15)

Let us stress that this analytical solution from the stability analysis, gives the wavelength of the fastest growing mode at the beginning of the ripple evolution (when nonlinear terms have small effects). We verified numerically that, at the beginning, the periodic instabilities have typical wavelengths which are close but not identical to \(\hat{\lambda}\) (equation (15)), observing typical wavelengths which are between 10 and 30% smaller than \(\hat{\lambda}\). For instance, in the simulation reported in figure 6 (see next section for details) the surface initially undulates with wavelengths \(\lambda \sim 51\), whereas equation (15) predicts \(\hat{\lambda} \simeq 55\). Note that equation (15) gives the fastest growing mode but the spectrum of instability is much wider having unstable modes for \(0 < k < k^*\), which correspond to wavelengths larger than \(2\pi/k^*\). From equation (12) we have \(k^* \simeq \sqrt{2} \hat{k}\), therefore the predicted range of possible unstable modes is \(\hat{\lambda}/\sqrt{2} < \lambda < \infty\), a range which is consistent with the numerical observations.

5.3. Some special cases

Let us first observe that, when \(K_1, s_1\) and \(\phi\) are equal to zero, the expression for the ripple wavelength, given by equation (15), coincides with the expression for sand dunes in deserts (see for instance [24]). In our notation the ‘reptation length’ is \(l_0 = v/\gamma\), the ‘cut-off length’ is \(l_c = (D_2 - D_1)/v\), whereas \(v_1 - v_2\) is the collective drift velocity of the dunes. The approximations...
Figure 6. (a) Evolution of the periodic ripples’ amplitude ($w = \text{root mean square of the height profile}$) (log scale) versus time (linear scale) from numerical simulations (arbitrary units; see appendix D). The four different behaviours are obtained by changing the numerical noise from $\epsilon = 10^{-8}$ to $10^{-12}$. The inset (b) are the same plots in log–log scale. When the Erlich–Schwoebel barrier is active the dynamical evolution of the ripples’ amplitude shows an exponentially fast growth at the beginning followed by a ‘saturation’ to a slower growth. This last regime shows a complex behaviour characterized by continuous re-nucleation and interaction of ripples. See appendix D for details on the parameters used in the simulation.

usually applied in this context [23, 24], imply: $l_c \gg \sqrt{D/\gamma}$, and $\gamma l_c \gg v_1 - v_2$, giving, from equation (15)

$$\hat{\lambda} \sim 2\pi \sqrt{\frac{2vl_0l_c}{v_1 - v_2}}.$$  

(16)

Let us now consider the dynamical evolution of a surface under ion bombardment and in particular the case when the effect of the Erlich–Schwoebel barrier is not present (as in semiconductors and glasses). In this case, $s = 0, s_1 = 0$ and we also expect that the drift velocity $v$ and the dispersion constant $D$ are equal to zero or infinitesimally small. Indeed, here the current of mobile atoms on the surface is mainly induced by the differences in the chemical potential. Under these assumptions, from equation (15), the expression for the wavelength of the most unstable ripple is

$$\hat{\lambda} \sim 2\pi \sqrt{\frac{2k}{\nu}},$$  

(17)

where we called $v = \frac{\nu}{\eta} D_1 \phi / (1 - \phi)$, a quantity which plays the role of an effective surface tension. Note that equation (17) is the same result as from the Bradley and Harper theory [28, 30, 35, 39, 40].

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When the Erlich–Schwoebel barriers are active \((s, s_1 \neq 0)\), the wavelength for the fastest unstable mode is modified as follows:

\[
\hat{\lambda} \sim 2\pi \sqrt{\frac{2K}{v + s}}.
\]  

\(\text{(18)}\)

5.4. Orientation

The most unstable mode is selected by the position of the deepest minimum in the \((k_x, k_y)\) plane. Equation (14) gives the radial position \(|k| = \hat{k}\) at which a section of \(\text{Im}(\omega(k))\) along a given direction of \(k\) has a minimum. The azimuthal position \(\alpha\) of the absolute minimum is along the direction at which \(\text{Im}(\omega(k))\) reaches the most negative value (see figures 5 and B.1). In equation (7) we have different sources of orientation anisotropy, and in particular the terms \(D_1\) and \(D_2\) and the quantities \(v, v_1, v_2\), which are all dependent on the azimuthal angle. Consequently, we expect the formation of ripples along preferential directions when \(b_y, b_y\) and/or \(d_x, d_y\) are anisotropic and/or when the parameters \(v, v_1, v_2\) are different from zero. Physically, the anisotropy can be caused by off-normal ion sputtering or/and by the crystalline orientation.

6. Exact solutions

Compact analytical expressions for the values of \(k\) at which \(\text{Im}(\omega) = 0, (k^*)\) can be calculated from equation (7) in some special cases.

In particular, in the absence of deterministic and non-deterministic diffusions and without Erlich–Schwoebel barriers (when \(\phi = 0, s_1 = 0, K_1 = 0\) and \(D = 0\)), we obtain

\[
k^* = |k^*| = \sqrt{\frac{\gamma(v_1 - v_2)}{(v - v_1 + v_2)(D_2 - D_1)}},
\]  

\(\text{(19)}\)

where \(v, v_1\) and \(v_2\) are the components of \(v, v_1\) and \(v_2\) in the direction of \(k^*\).

On the other hand, when the excavation and re-adsorption are independent of the curvature \((K_1, s_1, D_1\) and \(D_2\) are zero), we find

\[
k^* = \sqrt{\frac{\gamma(v - \phi v_1)}{D(v_1 - v - (1 - \phi)v_2)}},
\]  

\(\text{(20)}\)

The effect of the deterministic diffusion induced by the chemical potential can be studied from the following solution:

\[
k^* = \sqrt{\frac{\phi \gamma D_1}{(1 - \phi)\gamma K_1 - D(D_1 - (1 - \phi)D_2)}},
\]  

\(\text{(21)}\)

which holds when \(v = 0, v_1 = 0, v_2 = 0, s_1 = 0\) and \(D = D_1 + (1 - \phi)D_2 > 0\).
However, when we set to zero \(v_1\), \(v_2\), \(D_1\) and \(D_2\), we find

\[
k^* = \sqrt{\frac{s_1}{K_1}},
\]

which implies that the uphill current due to the Erlich–Schwoebel barrier can generate instability even when the shape-dependent erosion and recombination terms are inactive.

### 7. Numerical solutions

In order to explore the kind of surface patterns that can be generated by ion bombardment and in order to study the dynamical evolution of such patterns, several numerical solutions of equation (1) have been investigated. The details about these simulations are reported in appendix D. Here, we focus on three main emerging facts: (i) surface ripple can rotate by varying the incident angle of the ion flux; (ii) different kinds of surface patterns can be generated by tuning the parameters; and (iii) after the initial exponential growth different stabilization and saturation regimes are observed.

#### 7.1. Ripple-rotation

We simulate the formation of surface patterns in amorphous materials, semiconductors and metals. In all these systems we observe that a rotation of the ripple orientation can be induced by changing the relative weights of the coefficients \((b_x, b_y)\) with respect to the coefficients \((d_x, d_y)\). Experimentally, these coefficients can be varied by changing the angle \(\theta\) between the incident ion flux and the normal to the surface (it has been shown [28] that for oblique incidence the parameters \(b_x, b_y\) are proportional to \(\sin \theta\)). Moreover, the relative weights of these parameters depend on the temperature and, in metals, crystalline anisotropy might induce preferential directions.

In figure 7 is shown an example of 90° degrees ‘ripple-rotation’ in a metal (where the Erlich–Schwoebel barrier is active). A similar rotation in a system with no Erlich–Schwoebel barrier is shown in figure 8. Details on the used parameters are given in appendix D. For a further discussion of the orientation-dependence of the instability modes see appendix B.

#### 7.2. Different kinds of surface patterns

The emergence of different kinds of self-organized surface patterns has been explored numerically showing that the system parameters can be tuned in order to generate not only periodic ripples but also several other kinds of regular and periodic shapes. Figure 9 gives some examples of observed patterns. Experimentally, such a ‘tuning’ of the parameters can be performed by changing the orientation and intensity of the ion flux and/or by changing the temperature. In appendix D further details on such simulations are given.

#### 7.3. Exponential growth, stabilization, saturation and critical roughness

In metals, when the Erlich–Schwoebel barrier is active, there is an important nonlinear contribution in the current of mobile atoms which becomes sizable when the roughness (root mean square of the height profile) becomes sufficiently large and therefore \(\langle (\alpha_d \nabla h)^2 \rangle \sim 1\) (see
Figure 7. An example of ripples rotation (Erlich–Schwoebel barrier active—metals) associated with the change in the orientation of the ion flux (corresponding to a change in the relative weight of the coefficients $(b_x, b_y)$ in respect to $(d_x, d_y)$, see appendix D for details).

Figure 8. An example of ripples’ rotation (top and bottom) in semiconductors (no Erlich–Schwoebel barrier) associated with the variation of the relative weights of the parameters $(b_x, b_y)$ with respect to $(d_x, d_y)$, see appendix D for details.

equation (4)) (the average is over the surface positions). We observe, numerically that this term changes the ripple’s growth dynamics: from exponential to a slower growth which is initially consistent with a power-law growth and then it slows further down to a complex behaviour with different dynamical regimes which follow an overall logarithmic trend. In this saturation regime the ripple wavelength also tends to grow with time. We observe that this saturation regime is affected by the presence or the absence of a noise term in equation (2). In particular, in the absence of noise we can observe a saturation to a fixed profile with constant roughness. A theoretical justification of this regime is under current investigation, further details on the simulations are given in appendix C. From these preliminary studies it seems apparent that this
Figure 9. Ripples can rotate or a different kind of profile instability can form when the components of the parameters $v, v_1, v_2$ vary in the $(x, y)$ plane (left and right figures) or they are set to zero (central figure). See appendix D for further details.

The phase of the growth is characterized by a strong nonlinearity with a strong dependence of the ripple shapes (figure 10) and dynamic (figures 6) on small variations of the system parameters or the starting conditions. These preliminary studies seem to indicate that this regime is governed by the re-nucleation of new instabilities over the rippled surface. Experimentally, power-law growth of the roughness and growth of characteristic wavelengths were observed in erosive sputtering [7]. On the other hand, re-nucleation of instabilities has not yet been reported.

In semiconductors or glasses, when no Erlich–Schwoebel barrier is present, it is physically intuitive that the exponential growth of the surface roughness (which is a characteristic of the beginning of the surface instability) cannot continue indefinitely. Indeed, from the expression $R(r, t) = R_0 + \hat{R}_1 \exp(i\omega t + ikr)$, which we used to derive equation (15), we can immediately observe that when $\hat{R}_1 > R_0 = (1 - \phi)\eta/\gamma$, the amount of mobile atoms might become negative. Since a negative amount of atoms is physically impossible, the process of exponential growth of the roughness must necessarily terminate around a critical roughness given by

$$W_c \sim (1 - \phi)^{\eta/\gamma}.$$  (23)

This behaviour is confirmed by numerical solutions of equation (1) and it is expected to be observable in semiconductors and glasses after sufficiently long times.

We note that in the present section, these nonlinear effects are only sketched and this might lead to some incompleteness and trivialities. A systematic study of the nonlinear behaviour is a worthwhile exercise which requires further careful investigations and it would be the subject of future publications.

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4 Numerically, we observe the appearance of infinitesimal negative values of $R(r, t)$. If these unphysical negative values are forced to zero, the exponential growth of the roughening interrupts.
Figure 10. During the exponential growth, the profile shows a typical sinusoidal shape (a). Whereas at the saturation/stabilization, the profile tends to eliminate the curvature creating more triangular-like shapes (b). At this stage, instabilities might take place, with short-wavelength profile corrugations which nucleate on the triangular-like profile (c). In this regime, the ripples’ amplitude grows slower than exponential and the ripple wavelength increases with time (see text).

8. Conclusions

We have shown that the same theoretical approach introduced to describe the formation of aeolian sand ripples can be conveniently applied to the study of the formation of periodic structures on surfaces under ion sputtering. Ripples in sandy deserts and ripples on ion-bombarded surfaces are two physically different phenomena where different particles are excavated, adsorbed and displaced on the surface by different physical agents. The equations used to describe the excavation and adsorption mechanisms (equations (2) and (3)) are the simplest expressions that take into account a dependence of these phenomena on the surface shape.

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Indeed, they are composed by a constant term, plus a first derivative, plus a second derivative (i.e. height/orientation, slope and curvature). Such terms must appear in any theory that addresses the problem of surface excavation and adsorption. On the other hand, the mobility term contains more specific contributions, like the deterministic diffusion or the Erlich–Schwoebel barrier, which are specific of the ion-sputtering surface physics. But, also in this case, they describe a rather simple dependence of the particle mobility on the surface shape. Similar terms might be profitably introduced in the description of sand-dune dynamics.

We performed a linear stability analysis for pattern formation under sputtering erosion and we obtained general expressions for the wavelengths of the most unstable modes in terms of the system parameters. We show that in some particular cases such solutions coincide with the ones already known in the literature for sand dunes and surface instability [23, 24, 28, 30, 32]. We have discussed the effect of the Erlich–Schwoebel barriers and compared the result with numerical solutions. We pointed out that the Erlich–Schwoebel barrier can be responsible for a dramatic change in the system dynamics: from the exponential growth to a slower growth initially compatible with a power-law dynamics. The occurrence of a critical roughness has been predicted. The effect of ripple re-nucleation in this regime has been also highlighted. The dependence of the ripple orientation and shapes on the ion beam orientation and intensity has been discussed and the intriguing phenomenon of ‘ripple-rotation’ as well as the formation of other self-organized patterns have been accounted.

It should be noted that the main purpose of this paper is to point out a relevant example of universality: two processes which have completely different scales present a dynamical evolution which obeys to the same geometrical constraints and thus can be described by using the same phenomenological model. On the other hand, we must observe that the class of solutions of equation (1) is rich and complex—even in the linear approximation. Exhaustive, systematic studies of the classes of solutions of this equation and their dependence on the set of parameters will be the subject of future studies.

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Appendix A. Fourier transform of the linearized equation

By substituting equations (2), (3), (4) and (5) into equation (1) and by neglecting the second-order terms (in $R_1$ and $h_1$), we obtain the following linearized equation:

$$
\frac{\partial h_1}{\partial t} = \gamma R_1 - [v_1 - (1 - \phi)v_2] \nabla h_1 - [D_1 - (1 - \phi)D_2] \nabla^2 h_1,
$$

$$
\frac{\partial R_1}{\partial t} = -\gamma R_1 - v \nabla R_1 + D \nabla^2 R_1 + (1 - \phi)[(v_1 - v_2) \nabla h_1 + (D_1 - D_2 - s_1) \nabla^2 h_1 - K \nabla^4 h_1].
$$

(A.1)
A Fourier analysis of equation (A.1) leads to

\[
\gamma \hat{R}_1 - \left\{ i \omega + i k \left[ \mathbf{v}_1 - (1 - \phi) \mathbf{v}_2 \right] - k^2 \left[ D_1 - (1 - \phi) D_2 \right] \right\} \hat{h}_1 = 0,
\]

\[
\left[ i \omega + \gamma + i k \mathbf{v} + k^2 D \right] \hat{R}_1 - (1 - \phi) \left[ i k (\mathbf{v}_1 - \mathbf{v}_2) - k^2 \left( D_1 - D_2 - s_1 \right) \right] \hat{h}_1 = 0, \quad (A.2)
\]

with \( \hat{R}_1 \) and \( \hat{h}_1 \) the Fourier components of \( R_1 \) and \( h_1 \) respectively. This equation is a simple linear equation in two variables. It admits a non-trivial solution when the determinant of the coefficients is equal to zero. This leads to equation (6).

Appendix B. Orientation dependence of the instability

There are three distinct mechanisms that can lead to ‘ripple-rotation’ and the formation of other self-organized periodic patterns.

The first is associated with the anisotropies in the curvature-dependent erosion coefficients \( b_x, b_y \) and in the curvature-dependent adsorption coefficients \( d_x, d_y \). These anisotropies are induced both by the sputtering orientation angle and by the crystal orientation (in non-amorphous surfaces). In particular figures 7 and 8 show that a 90° degrees rotation in the ripple orientation can be induced by varying the angle of the incident ion flux.

The second mechanism which can induce ripple-rotation is associated with the vectorial terms \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \). In figure B.2 are plotted various solutions of equation (6) for the branch of \( \text{Im}(\omega) \) which can admit negative values. The plot is \( |k| \) versus \( \text{Im}(\omega) \) along a given azimuthal direction. In figure B.2(a), we show the weakening and disappearance of the negative minima in a given direction caused by the increase in the component of \( \mathbf{v}_1 \) along this direction. In figure B.2(b), we show the re-appearance of the negative minima by increasing the component of \( \mathbf{v}_2 \) along the same direction, whereas in figure B.2(c), the minima are recovered by decreasing simultaneously the components of both \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \) along this direction. (In these plots we used: \( \gamma = 1, \phi = 0.5, v = 2, D = 0.1, K_1 = 0.4, s_1 = 7, D_1 = 0.7 \) and \( D_2 = 1 \). Figure B.2(a) varies \( v_1 \) between 4 and 100 at fixed \( v_2 = 1 \). Figure B.2(b) fixes \( v_1 \) at 100 and increases \( v_2 \) from 10 to 98. Figure B.2(c) decreases \( v_1 \) from 100 to 2 and decreases \( v_2 \) from 1 to 0.02.)

Another example is given in figure B.1 where the position of the minimum rotates by ~90° by changing the components \( x, y \) of the coefficient \( v_1 \).

The third mechanism which influences the orientation of the ripples is associated with the drift velocity \( \mathbf{v} \). We expect this last mechanism to be more relevant in the case of aeolian dunes and less important in ion-sputtered surfaces.

What we want to stress is that the phase diagram associated with these solutions is very rich and highly non-trivial. Instabilities in a given direction can be triggered on and off by changing the relative weights of the quantities \( b_x, b_y \) or \( d_x, d_y \) or by varying the intensities or the components of the parameters \( \mathbf{v}, \mathbf{v}_1, \mathbf{v}_2 \). These changes are associated with variations of the normal and azimuthal orientations of the ion sputtering, with changes in the intensity of the ion flux, with the variation of the temperature of the substrate, and with several other physical changes in the experimental set-up. It is beyond the purpose of the present paper to discuss in detail these aspects; however, we want to make clear that the present theory can account for these phenomena.
Figure B.1. Surface plot and contour lines plot for the imaginary part of the dispersion relation \( \text{Im}(\omega) \) from the analytical solution of equation (6) in the two-dimensional case. Figures (a) and (b) show the occurrence of a 90° rotation in the orientation of the instability mode associated with the variations of the components in the \( x, y \) plane of the coefficient \( v_1 \). (The plots on the left side have parameters: \( v_x = 0.1, v_y = 0.1, (v_1)_x = 10, (v_1)_y = 0.001, v_2 = 0, s = 7, \gamma = 1, \eta = 1, D = 0.1, D_1 = 0.7, D_2 = 1, K_1 = 0.4, \phi = 0.2 \). The right plots use the same parameters with exchanged components for \( v_1 \).)

Appendix C. Saturation/stabilization

We have observed numerically that the behaviour of the surface instability in the saturation/stabilization regime described, in section 7.3, is very sensitive to the presence of a noise term added to equation (2) (see main text). In order to investigate this effect we have performed several simulations by varying the amplitude (\( \epsilon \)) of an additive Gaussian noise with average zero and variance \( \epsilon^2 \). Such a parameter \( \epsilon \) was varied from zero to an upper limit which has been chosen several order of magnitudes smaller of the critical roughening \( W_c \). We observe that the stabilization/saturation dynamics is affected by the amplitude of the additive noise. In particular,
Figure B.2. The imaginary part of the dispersion relation $\text{Im}(\omega)$ versus $|k|$ along 
a given azimuthal direction for various values of the components of $\mathbf{v}$, $\mathbf{v}_1$, $\mathbf{v}_2$. Instabilities become deeper or rise and even disappear depending on the relative 
weights of the components of $\mathbf{v}$, $\mathbf{v}_1$, $\mathbf{v}_2$ (see text).

in some regions of the parameters, we observe that the saturation to a constant roughening can 
be achieved only in the absence of noise contribution. But it must be noted that the observed 
behaviours are extremely complex and show a strong dependence on the starting configuration, 
on the history (time steps, random generated noise, etc) and on the system parameters. After all, 
this is not surprising in a nonlinear system.

Let us here briefly describe the kind of (nonlinear) dynamics that we observe numerically 
in the one-dimensional case. When the Erlich–Schweoebel barrier is active, after the first 
exponential growth, the system reaches a saturation/stabilization regime where the roughening 
grows slower than exponential or stays constant. In the exponential growth stage, we observe 
that the surface profile has a typical sinusoidal-like shape (see figure 10(a)). After this stage, at 
the saturation/stabilization regime the surface tends to assume a triangular-like profile flattening 
in this way its curvature and concentrating it at the vertices (figure 10(b)). In this regime, the 
growth of the surface-ripples might end or, vice versa, it might re-start from small instabilities 
(infinitesimal noise) generated over the triangular shapes (figure 10(c)). In this second case, the 
re-nucleated ripples follow a similar history of the ones on which they nucleate: they start with an 
exponential growth and then reach a saturation until another re-nucleation occurs. In this phase, 
interactions among ripples nucleated in different parts of the surface, and the interaction between 
the newly nucleated ripples and the pre-existent surface corrugations play a major role. Typically, 
the overall dynamics shows an initial power-law growth associated with a change in the ripple 
wavelength then this growth slows down further, becoming consistent with a logarithmic overall 
trend. But, it should be noted that, a finer analysis of this process shows a complex non-uniform 
growth.

(Figures 10(a) and (b) were generated by setting: $v = 0.1$, $D = 0.2$, $K = 3$, $s = 0.6$, 
$\phi = 10^{-5}$, $\eta = 0.05$, $\gamma = 0.03$, $a = 1$, $b = 5$, $c = 0.1$, $d = 0.5$, $\alpha = 10^5$, with no additive 
noise; whereas figures 10(c) has the same set of parameters but with an infinitesimal additive 
Gaussian noise $\epsilon$ (equation (2)) with zero mean and standard deviation equal to $10^{-11}$.)

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Appendix D. Numerical solution parameters

The numerical solutions of equation (1) presented in this paper, and in particular the ones shown in figures 2 and 6, have been performed as follows. We considered a one-dimensional flat substrate \((h(x, 0) = h_0)\) of length \(L\), with periodic boundary conditions. An infinitesimal quantity of mobile atoms were added randomly to the substrate (with \(0 < R(x, 0) < L/N10^{-13}\)). We have then computed the profile evolution by using equation (1) with the derivative substituted with finite differences. To this purpose, the substrate has been divided into \(N\) discrete points. The adimensional time indicated in figure 6 is the number of steps. The lengths are in units of \(l_0 = L/N\) and the roughness is defined as \(w(t, L) = \langle h(x', t) - \langle h(x, t)\rangle_x \rangle^2_x^{1/2}\) (see, for instance [33]).

Several computations with the number of points equal to \(N = 1000, 2000\) and 3000 (the one presented here have \(N = 3000\)) have been performed to verify the effect of boundary and discretization. Moreover, simulations with no periodic boundary conditions and with the ion-bombardment term (equation (2)) applied only to a central mask, have also been performed obtaining very similar results. The robustness of the present approach has been verified varying the parameters, the time steps, the initial roughness of the substrate, etc. Comparable results have been always found, but we must stress that, under some conditions, numerical instabilities (in particular surface deformations with \(\lambda \sim L/N\)) can arise depending on the protocol utilized.

(The simulation results, shown in figures 2 and 6, use: \(v = 0.1, D = 0.2, \mathcal{K} = 3, s = 0.6, \phi = 10^{-5}, \eta = 0.05, \gamma = 0.03, a = 1, b = 5, c = 0.1, d = 0.5, \alpha = 10^8\), with the noise term equal to zero (figure 2) or varying between \(10^{-8}\) and \(10^{-12}\) (figure 6). The simulation time was up to \(10^6\) steps.)

The numerical solutions for the two-dimensional case have been calculated by following the same protocol as in the one-dimensional case. In two dimensions the substrate is a square \(L \times L\) surface with periodic boundary conditions which has been subdivided into a discrete grid of \(150 \times 150\) points. (The simulation result shown in figure 3 uses \(v = 0, D = 0, \mathcal{K} = 0.5, s = 0, \phi = 0.2, \eta = 0.05, \gamma = 0.03, a = 0, b_x = 2, b_y = 5.\) The simulations in figure 7 use \(v = 0, D = 0.5, \mathcal{K} = 0.5, s = 0.6, \phi = 0.1, \eta = 0.5, \gamma = 0.03, a = 0, c = 0, d_x = 0.3, d_y = 0.3, \alpha = 0.\) The simulations in figure 8 use \(v = 0, D = 0.5, \mathcal{K} = 0.5, s = 0.6, \phi = 0.2, \eta = 0.05, \gamma = 0.03, a = 0, c = 0, d_x = 0.3, d_y = 0.5, \alpha = 0,\) with the top and bottom figures generated respectively by using \((b_x, b_y) = (0.8, 0.05)\) and \((0.5, 0.5).\) The simulations in figure 10 use \(v = 0, D = 0.5, \mathcal{K} = 0.5, s = 0.6, \phi = 0.2, \eta = 0.05, \gamma = 0.03, a = 0, c = 0, d_x = 0.3, d_y = 0.5, \alpha = 0,\) with the top and bottom figures generated respectively by using \((b_x, b_y) = (6, 10)\) and \((5, 6).\) The noise was \(\epsilon = 10^{-10}\) for all the two-dimensional simulations. The simulation times were up to 30000 steps.)

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