

SURFACE DIFFUSION INCLUDING ADATOMS*

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Abstract. The aim of this paper is to study continuum models for surface diffusion taking into account free adatoms on the surface, which is of particular importance in the (self-assembled) growth of nanostructures. The extended model yields a coupled system of parabolic differential equations for the surface morphology and the adatom density, involving a cross-diffusion structure.

We investigate two different situations, namely the growth of a film on a substrate and the growth of a crystal-like structure (a closed curve or surface). An investigation of the equilibrium situation, which can be phrased as an energy minimization problem subject to a mass constraint, shows a different behaviour in both situations: for the film the equilibrium is attained when all atoms are attached to the surface, while for a crystal the adatom density does not vanish on the surface. The latter is also a deviation from the usual equilibrium theory, since the equilibrium shape will be strictly included in the Wulff shape. Moreover, it turns out that the total energy is not lower semicontinuous and non-convex for large adatom densities and rough surfaces.

The dynamics of the adatom surface diffusion model is investigated in detail for situations close to a flat surface in the film case and the situation close to a radially symmetric curve, both with an almost spatially homogeneous adatom density, where the cross-diffusion structure of the model and the decay to equilibrium can be studied in detail. Finally, we discuss the numerical solution of the adatom surface diffusion model in the film case and provide various simulation results.

Key words. Surface Diffusion, Nanostructure Growth, Numerical Simulation

AMS subject classifications. 74N20, 74N25, 35K50, 35K55, 65M60

1. Introduction

Surface diffusion is one of the most important growth mechanisms in nanoscale surface growth and modern materials science (cf. [51]). Though the basic growth laws were known for several decades after they have been derived by Mullins [40] in the modelling of thermal grooving, strong interest in the theory and simulation of surface diffusion has been initiated recently, driven by applications to electromigration of voids (cf. e.g. [2, 3, 35]), shape transition in alloys (cf. [16]) and in particular, by the growth of nanostructures (cf. [27, 34, 44, 45, 47, 50]).

The standard model of isotropic surface diffusion is given by a geometric motion law for a surface $\Gamma(t)$:

$$-\operatorname{div}_S(L\nabla_S\mu) + \rho V = \mathbf{r} \cdot \mathbf{n} \quad (1.1)$$

$$-\psi\kappa - \rho\mu = 0, \quad (1.2)$$

on $\Gamma(t)$. The unknowns in this system are the chemical potential μ and the surface $\Gamma(t)$, with its outer unit normal \mathbf{n} , its mean curvature $\kappa = \operatorname{div} \mathbf{n}$, and its normal velocity V , given by

$$V = \frac{\partial \mathbf{x}}{\partial t} \cdot \mathbf{n}, \quad \mathbf{x} \in \Gamma(t). \quad (1.3)$$

The vector \mathbf{r} denotes a deposition flux to the surface, L is the mobility of atoms on the surface, ψ the (constant) free energy, and ρ is the material density. The subscripts S

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in the differential operators are used to denote derivatives with respect to the surface variables S .

The surface diffusion model (1.1), (1.2) and extensions to anisotropic situations have been discussed with respect to modelling aspects (cf. e.g. [5, 13, 17, 41]), analysis (cf. e.g. [4, 8, 10, 24, 25, 38]), and numerical simulation (cf. e.g. [6, 7, 14, 15, 18, 32, 39, 45, 49]). The main properties of surface diffusion are the dissipation of the surface energy

$$E(\Gamma(t)) = \int_{\Gamma(t)} \psi \, dS \quad (1.4)$$

via

$$\frac{d}{dt} E(\Gamma(t)) = - \int_{\Gamma(t)} |\nabla_S \mu|^2 \, dS, \quad (1.5)$$

and conservation of the volume (respectively the mass for constant bulk density), i.e.,

$$\frac{d}{dt} \int_{\Omega(t)} \rho \, d\mathbf{x} = 0. \quad (1.6)$$

Surface diffusion is usually treated as a fourth-order evolution equation for some variables representing the surface, which somehow shadows the physical interpretation of the model. The first equation (1.1) actually models the diffusion of atoms along the surface, while (1.2) determines the attachment and detachment process. In many cases, e.g. in vapour deposition processes, it is important to include adatoms ("attached atoms") into the model, which freely diffuse on the surface. Moreover, it is often important to model kinetic effects appearing in the attachment process.

If adatoms and kinetic effects are included, the model changes to (cf. [26] and Section 2.1)

$$\frac{\partial \delta}{\partial t} - \operatorname{div}_S(L \nabla_S \mu) + (\rho - \delta \kappa) V = \mathbf{r} \cdot \mathbf{n} \quad (1.7)$$

$$bV - \psi \kappa - (\rho - \delta \kappa) \mu = 0, \quad (1.8)$$

where δ denotes the adatom density, b is a kinetic coefficient. For the sake of simplicity, we shall consider b as well as the diffusion coefficient L and the bulk density ρ to be positive constants throughout the paper. The free energy in this case depends on the adatom density, and the chemical potential μ is determined by

$$\mu = \psi'(\delta), \quad (1.9)$$

which corresponds to the original interpretation of the chemical potential as the free energy variation when atoms are attached to or detached from the surface. The term

$$\rho^{\text{ef}} = \rho - \delta \kappa \quad (1.10)$$

can be interpreted as an effective density. If the adatom density is continued to be locally constant in normal direction, then the effective density corresponds to the variation of the total mass

$$m(\Gamma, \delta) = \int_{\Gamma} \delta \, dS + \int_{\Omega} \rho \, d\mathbf{x} \quad (1.11)$$

with respect to local surface variations. The surface energy of the system is now a functional of the surface and of the adatom density, i.e.,

$$E(\Gamma, \delta) = \int_{\Gamma} \psi(\delta) \, dS. \quad (1.12)$$

The analysis and numerical simulation of the surface diffusion model (1.1), (1.2) is still a subject of ongoing research, but there exists a variety of results that contribute to the understanding of the dynamics. The equilibrium problem related to classical surface diffusion, namely the minimization of the surface area (or anisotropic versions of the surface energy) subject to a volume constraint seems to be completely understood nowadays. For the adatom surface diffusion model (1.7), (1.8), which is certainly of practical importance and may even model the ongoing surface physics more accurately, the situation is different. To our knowledge there are neither analytical nor numerical results about the dynamics available, and even the corresponding equilibrium problem seems not to be well-understood. The aim of this paper is a detailed analytical and numerical study of the adatom surface diffusion model (1.7), (1.8), which hopefully contributes to the further understanding of surface diffusion processes. We shall study the model for surfaces in \mathbb{R}^3 , with obvious physical interpretation, as well as for curves in \mathbb{R}^2 (sometimes called edge diffusion), which can be applied e.g. to adatom diffusion along islands in epitaxial growth (cf. [12]).

The main results we shall obtain below are the following:

- Convexity of the surface energy for small adatom densities and sufficiently flat surfaces, and non-convexity of the surface energy for larger adatom densities and in particular for rough surfaces, which is a significant difference to models ignoring free adatoms, where the surface energy is globally convex in isotropic and weakly anisotropic situations.
- In the case of films growing on substrates, the global equilibrium is obtained for a flat surface and vanishing adatom density, which clearly is the same one as without modelling free adatoms. In the case of structures growing in the bulk, the equilibrium is different, in particular the Wulff shape with vanishing adatom density is not an equilibrium when adatom densities are included in the energy model.
- The dynamics of the model changes from a fourth-order parabolic evolution equation to a coupled system of two second-order parabolic evolution equations with cross-diffusion structure. This structure is studied in detail by asymptotic expansions around flat surfaces and spherical shapes with constant adatom densities. Moreover, by linearization around such special structures and arguments based on the implicit function theorem, we are able to provide existence results in some situations. In addition, we derive exponential decay to equilibrium for smooth nonnegative solutions in the case of a film growing on a substrate.
- We introduce a numerical scheme based on finite element discretization in space and a semi-implicit time-stepping, which allows us to compute approximations to the nonlinear adatom surface diffusion model by solving a stable linear system in each time step.

The paper is organized as follows: in the remainder of this section we introduce the basic notations and review the definition of function spaces used throughout the paper. In Section 2 we introduce some basic formulations of adatom surface diffusion and provide a formal discussion of the relation to the classical surface diffusion

model. Section 3 is devoted to the study of equilibrium structures, starting with an investigation of the surface energy and its convexity properties, and continuing with the explicit computation of the global equilibria and the characterization of stationary points. In Section 4 we study the dynamics by adatom surface diffusion close to important special situations, provide an existence result for initial values close to flat films, and verify the exponential decay of the energy and the adatom density for films. A derivation of a fully discrete scheme for the numerical simulation in the film case is provided in Section 5, as well as several simulation results illustrating the nonlinear dynamics. Finally, we conclude in Section 6.

1.1. Notation. The basic notation used in this paper is as follows: by \mathbf{x} we denote spatial variables in \mathbb{R}^d or \mathbb{R}^{d+1} and by x_i their components. The time variable is denoted by t in general, and surface variables are denoted as S . For surfaces (or curves) we always use the notation Γ and for domains (partly) bounded by Γ the notation Ω . Moreover, we shall use the notation D for a rectangular domain of the form $D = \prod_{i=1}^d (-d_i, d_i)$, for $d_i \in \mathbb{R}_+$.

The geometric quantities used frequently in the following are the unit outer normal \mathbf{n} (i.e., the normal pointing into $\mathbb{R}^{d+1} \setminus \Omega$) and the mean curvature κ . The total velocity of a boundary point is denoted by \mathbf{V} , the normal velocity by $V = \mathbf{V} \cdot \mathbf{n}$, and the tangential velocity by $\mathbf{v} = \mathbf{V} - V\mathbf{n}$.

Partial derivatives of a function f with respect to variable y are denoted by $\frac{\partial f}{\partial y}$, as the gradient ∇f we denote the vector of partial derivatives with respect to the spatial variables (and not the time variable), and similarly the divergence with respect to spatial variables is denoted by $\operatorname{div} f$. If a gradient or divergence is taken with respect to the surface variables we use a subscript S , i.e. $\nabla_S = (I - \mathbf{n} \otimes \mathbf{n})\nabla$ and div_S .

1.2. Function spaces. Throughout the whole paper we shall use standard notation for function spaces. For a domain $M \subset \mathbb{R}^m$ we denote by $C(M)$ the space of continuous functions on M equipped with the supremum norm. By $C^k(M)$, $k \in \mathbb{N}$ we denote the space of k -times continuously differentiable functions equipped with the norm (using standard multi-index notation)

$$\|f\|_{C^k} = \max_{\alpha \in \mathbb{N}^m, |\alpha| \leq k} \left\| \frac{\partial^\alpha f}{\partial \mathbf{x}^\alpha} \right\|_{C^0}.$$

By $L^p(M)$, $p \in [1, \infty)$ we denote the Lebesgue space of measurable p -integrable functions, with the norm

$$\|f\|_{L^p} = \left(\int_M |f(\mathbf{x})|^p d\mathbf{x} \right)^{1/p},$$

and by $L^\infty(M)$ the space of measurable essentially bounded functions with the norm

$$\|f\|_{L^\infty} = \operatorname{ess\,sup}_{\mathbf{x} \in M} |f(\mathbf{x})|.$$

For $k \in \mathbb{N}$ and $p \in [1, \infty]$, we denote by $W^{k,p}(M)$ the Sobolev space of functions with distributional derivatives up to order k in $L^p(M)$, equipped with the norm

$$\|f\|_{W^{k,p}} = \left(\sum_{\alpha \in \mathbb{N}^m, |\alpha| \leq k} \left\| \frac{\partial^\alpha f}{\partial \mathbf{x}^\alpha} \right\|_{L^p}^p \right)^{1/p}$$

for $p \in [1, \infty)$, and

$$\|f\|_{W^{k,\infty}} = \max_{\alpha \in \mathbb{N}^m, |\alpha| \leq k} \left\| \frac{\partial^\alpha f}{\partial \mathbf{x}^\alpha} \right\|_{L^\infty}.$$

For the particular case $p=2$ we use the standard notation $H^k(M) = W^{k,2}(M)$, and we denote its dual space by $H^{-k}(M)$. We refer to [36] for detailed definitions of Sobolev spaces.

For M being of the form $M = \prod_{j=1}^m (m_j^-, m_j^+)$ we can define subspaces of all the spaces above including only periodic functions, as the closure of periodic functions of class C^∞ with mean value zero in the respective topology. These periodic spaces shall be denoted with an extra subscript *per*. In particular we have

$$L_{\text{per}}^p := \left\{ u \in L^p(M) \mid u \text{ periodic, } \int_M u \, d\mathbf{x} = 0 \right\}$$

and

$$W_{\text{per}}^{k,p} := \left\{ u \in W^{k,p}(M) \mid u \text{ periodic, } \int_M u \, d\mathbf{x} = 0 \right\}.$$

We shall also need spaces of vector-valued functions on a time interval $[0, T]$ with values in a Sobolev space $W^{k,p}(M)$. The space of continuous maps from $[0, T]$ into a Sobolev space $W^{k,p}(M)$ shall be denoted by $C(0, T; W^{k,p}(M))$. In an analogous way we define the spaces $C^k(0, T; W^{k,p}(M))$, $L^p(0, T; W^{k,p}(M))$ and $W^{\ell,q}(0, T; W^{k,p}(M))$. We refer to [37, 46] for details on vector-valued spaces for evolution problems.

2. Formulations and basic properties

In the following we briefly review the derivation of the model and discuss the basic geometric setup used in the cases of films and crystals growing by adatom surface diffusion. We shall introduce strong and weak formulations of (1.7), (1.8), and verify basic properties of the evolution such as energy dissipation and mass conservation.

2.1. Derivation of the model. Since the adatom surface diffusion model (1.7), (1.8) is not a standard model in literature, but has been derived only recently (cf. [26]) in a general setting, we briefly discuss its derivation in the case we are interested in.

Let $\Gamma_0(t) \subset \Gamma(t)$ be arbitrary and let $\Omega_0(t) \subset \Omega(t)$ be an arbitrary subdomain such that $\Gamma_0(t) = \partial\Omega_0(t) \cap \Gamma(t)$. Then the mass $m_0(t)$ contained in $\Omega_0(t)$ and at its boundary consists of inner atoms and atoms on $\Gamma_0(t)$, i.e.

$$m_0(t) = \int_{\Omega_0(t)} \rho \, d\mathbf{x} + \int_{\Gamma_0(t)} \delta \, dS.$$

If we ignore bulk diffusion but allow deposition and surface diffusion of adatoms, then change of mass in $\overline{\Omega_0(t)}$ is only due to deposition (with effective density $\mathbf{r} \cdot \mathbf{n}$) and flux of mass over the boundary of Γ_0 . If we use a standard diffusion law for the flux (equal to $L \nabla_S \mu \cdot \mathbf{N}_0$, where L is a mobility coefficient and \mathbf{N}_0 is the unit outer normal to $\Gamma_0(t)$ restricted on $\Gamma(t)$) we obtain

$$\begin{aligned} \frac{dm_0}{dt}(t) &= \int_{\Gamma_0} \mathbf{r} \cdot \mathbf{n} \, dS + \int_{\partial\Gamma_0} L \nabla_S \mu \cdot \mathbf{N}_0 \, ds \\ &= \int_{\Gamma_0} (\mathbf{r} \cdot \mathbf{n} - \text{div}_S(L \nabla_S \mu)) \, dS, \end{aligned} \quad (2.1)$$

where we have used Gauss' Theorem to rewrite the second term. In order to compute the time derivative of $m_0(t)$ we can apply standard results for derivatives of domain-dependent integrals (Theorem 4.2 in [20, p. 352] for the first and Theorem 4.3 in [20, p. 355] for the second one), which yields

$$\frac{dm_0}{dt}(t) = \int_{\Gamma_0} \rho V \, dS + \int_{\Gamma_0} \left(\frac{\partial \delta}{\partial t} + V \mathbf{n} \cdot \nabla \delta - \delta \kappa V \right) dS.$$

Since Γ_0 is arbitrary and δ can always be continued locally constant in normal direction, we can conclude the local equation (1.7) from (2.1), or, equivalently

$$\frac{\partial \delta}{\partial t} + V \mathbf{n} \cdot \nabla \delta - \operatorname{div}_S(L \nabla_S \mu) + (\rho - \delta \kappa) V = \mathbf{r} \cdot \mathbf{n} \quad (2.2)$$

if δ is not continued constant in normal direction away from $\Gamma(t)$, which will become important for representations of surfaces via graphs over a fixed domain.

We now consider the energy dissipation relation. Since the derivation in [26] is based on non-standard concepts such as configurational forces, we shall present a slightly different derivation here. For τ sufficiently small and a given normal velocity, let

$$\Gamma^\tau(t; V) := \{ \mathbf{x}(S) + \tau \mathbf{n}(S) \mid \mathbf{x}(S) \in \Gamma(t) \}.$$

By the principle of minimal work, the normal velocity on Γ is determined such that the work in an infinitesimal time interval ($\tau \rightarrow 0$) is minimized, i.e.,

$$\lim_{\tau \rightarrow 0} \left(W^\tau(t; V) - W^\tau(t; \tilde{V}) \right) \leq 0 \quad \forall \tilde{V},$$

where $W^\tau(t; \tilde{V})$ denotes the work needed to move $\Gamma(t)$ to $\Gamma^\tau(t; \tilde{V})$. This dissipation relation is equivalent to

$$\lim_{\tau \rightarrow 0} \frac{\partial W^\tau}{\partial V}(t; V) = 0.$$

The total work is the sum of work done by interfacial forces, mass transport and by kinetic forces. Using again the results on derivatives of shape functionals (cf. [20]), the work done by interfacial forces can be expanded as

$$W_1^\tau(t; V) = \frac{1}{\tau} (E(\Gamma^\tau(t; V), \delta) - E(\Gamma(t), \delta)) = - \int_{\Gamma(t)} \psi(\delta) \kappa \, dS + \mathcal{O}(\tau).$$

With $\Omega^\tau(t; V)$ denoting the domain with boundary $\Gamma^\tau(t; V)$ we obtain the work done by mass transport as

$$\begin{aligned} W_2^\tau(t; V) &= \frac{1}{\tau} \left(- \int_{\Omega^\tau(t; V)} \rho \mu \, d\mathbf{x} - \int_{\Gamma^\tau(t; V)} \delta \mu \, dS \right) \\ &\quad - \frac{1}{\tau} \left(- \int_{\Omega(t)} \rho \mu \, d\mathbf{x} - \int_{\Gamma(t)} \delta \mu \, dS \right) \\ &= - \int_{\Gamma(t)} (\rho - \delta \kappa) \mu V \, dS + \mathcal{O}(\tau). \end{aligned}$$

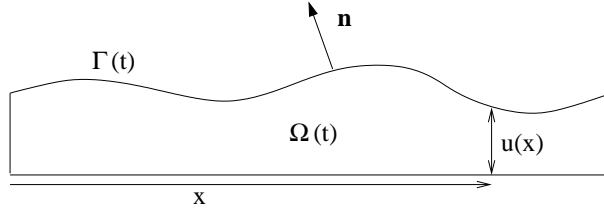


FIG. 2.1. Geometric setup in the case of a film growing by adatom surface diffusion.

Finally, the work of kinetic forces can be expanded in the usual way as

$$W_3^\tau(t; V) = \frac{b}{2} \int_{\Gamma(t)} V^2 dS + \mathcal{O}(\tau).$$

Hence, the energy dissipation becomes

$$0 = \frac{\partial}{\partial V} \left(- \int_{\Gamma(t)} \psi(\delta) \kappa V dS - \int_{\Gamma(t)} (\rho - \delta \kappa) \mu V dS + \frac{b}{2} \int_{\Gamma(t)} V^2 dS \right),$$

which yields (1.8).

We finally mention that the whole surface diffusion model can model a reasonable physical situation only when the adatom densities are reasonably small, since otherwise one would obtain a high number of free atoms diffusing not only along the surface, but also along a vapour phase. If δ is small, then we have to first order that

$$0 < \psi(0) \approx \psi(\delta) - \delta \mu.$$

As we shall see below, the stability condition $\psi - \delta \mu \geq 0$ also appears in the analysis at several instances.

2.2. Film growth. We start with a film on a substrate growing by surface diffusion. For the sake of simplicity, we restrict our attention to a periodic case and assume that the substrate covers the region $z < 0$. For a rectangular domain $D \subset \mathbb{R}^d$, $d = 1, 2$ we consider a film represented by its height function, i.e.,

$$\Omega(t) = \{ (\mathbf{x}, z) \mid \mathbf{x} \in D, 0 < z < u(\mathbf{x}, t) \}, \quad (2.3)$$

with the free surface

$$\Gamma(t) = \{ (\mathbf{x}, u(\mathbf{x}, t)) \mid \mathbf{x} \in D \}. \quad (2.4)$$

This setup is illustrated in Figure 2.1.

The unit outer normal is determined in terms of the height function as

$$\mathbf{n} = \frac{1}{Q} (-\nabla u, 1), \quad (2.5)$$

with the length of a surface element abbreviated by $Q = \sqrt{1 + |\nabla u|^2}$. The mean curvature and normal velocity of the surface are given by

$$\kappa = \operatorname{div} \left(\frac{\nabla u}{Q} \right), \quad V = \frac{1}{Q} \frac{\partial u}{\partial t}. \quad (2.6)$$

Finally we transform the surface divergence and gradient. It is well-known that the differential operator appearing in (1.1) and (1.7) can be written as (cf. e.g. [6])

$$\operatorname{div}_S(L\nabla_S\mu) = \frac{1}{Q} \operatorname{div}\left(L\frac{\mathbf{P}\nabla\mu}{Q}\right) \quad (2.7)$$

with the matrix

$$\mathbf{P} = Q^2\mathbf{I} - \nabla u \otimes \nabla u. \quad (2.8)$$

By representing the adatom density δ and the chemical potential μ as functions of $\mathbf{x} \in D$ and $t \in [0, T]$ and multiplication of the equations (2.2), (1.8) by Q , we obtain:

DEFINITION 2.1. *The strong formulation of the adatom surface diffusion model for film surfaces is given by the partial differential equations*

$$Q\frac{\partial\delta}{\partial t} - \operatorname{div}\left(L\frac{\mathbf{P}\nabla\mu}{Q}\right) + \frac{\partial u}{\partial t}\left(-\operatorname{div}\left(\delta\frac{\nabla u}{Q}\right) + \rho\right) + \nabla u \cdot \mathbf{r}_{12} = r_3 \quad (2.9)$$

$$b\frac{\partial u}{\partial t} - Q\operatorname{div}\left((\psi - \mu\delta)\frac{\nabla u}{Q}\right) - \delta\nabla\mu \cdot \nabla u - \rho\mu Q = 0 \quad (2.10)$$

in $D \times (0, T)$. A strong solution is a pair of functions

$$(\delta, u) \in W^{1,\infty}((0, T) \times D) \times L^\infty(0, T; W^{2,\infty}(D)) \cap W^{1,\infty}(0, T; L^\infty(D)),$$

satisfying (2.9), (2.10) as well as periodic boundary conditions and the initial conditions

$$\delta(\cdot, 0) = \delta_0, \quad u(\cdot, 0) = u_0 \quad \text{in } D. \quad (2.11)$$

Note that since the adatom density is not constant in normal direction in the graph representation we are using (2.2) in this case, and the effective density appearing in (2.9), (2.10) changes to

$$\rho^{\text{ef}} = \rho - \operatorname{div}\left(\delta\frac{\nabla u}{Q}\right). \quad (2.12)$$

By multiplication with test functions φ , w and subsequent integration by parts we derive the weak formulation of the adatom surface diffusion model in the film case, given by:

DEFINITION 2.2. *The weak formulation of the adatom surface diffusion model for film surfaces is given by the variational equations*

$$\begin{aligned} \int_D \left[\frac{\partial\delta}{\partial t} \varphi Q + L\frac{\mathbf{P}\nabla\mu \cdot \nabla\varphi}{Q} + \delta\frac{\nabla u}{Q} \cdot \nabla \left(\frac{\partial u}{\partial t} \varphi \right) + \rho \frac{\partial u}{\partial t} \varphi \right] d\mathbf{x} \\ = \int_D [r_3 - \nabla u \cdot \mathbf{r}_{12}] \varphi d\mathbf{x} \end{aligned} \quad (2.13)$$

$$\begin{aligned} \int_D \left[b\frac{\partial u}{\partial t} \frac{w}{Q} + \psi \frac{\nabla u \cdot \nabla w}{Q} - \delta \frac{\nabla u \cdot \nabla(w\mu)}{Q} - \rho w \mu \right] d\mathbf{x} \\ = 0 \end{aligned} \quad (2.14)$$

for all smooth periodic test functions $(\varphi, w) \in L^\infty(0, T; W^{1, \infty}(D))^2$, to be solved for periodic functions

$$(\delta, u) \in W^{1, \infty}(0, T; L^2(D) \times H^1(D)) \cap L^\infty(0, T; H^1(D) \times W^{1, \infty}(D))$$

satisfying the initial conditions (2.11).

We shall see below that the weak form is crucial for the construction of numerical schemes based on finite element discretizations.

By a suitable choice of test functions in (2.13), (2.14) one can verify the global energy dissipation

$$\begin{aligned} \frac{d}{dt} E(\Gamma(t), \delta(t)) &= \frac{d}{dt} \int_D \psi(\delta) Q \, d\mathbf{x} \\ &= - \int_D \left[L(\mathbf{P} \nabla \mu) \cdot \nabla \mu + b \left| \frac{\partial u}{\partial t} \right|^2 \right] \frac{1}{Q} \, d\mathbf{x} \\ &\quad + \int_D [r_3 - \nabla u \cdot \mathbf{r}_{12}] \mu \, d\mathbf{x} \end{aligned}$$

and global mass conservation

$$\frac{d}{dt} m(\Gamma(t), \delta(t)) = \frac{d}{dt} \int_D (\rho u + \delta Q) \, d\mathbf{x} = \int_D [r_3 - \nabla u \cdot \mathbf{r}_{12}] \, d\mathbf{x}$$

for all weak solutions and all $t \geq 0$. In particular it becomes clear that energy and mass are transported only through the deposition flux, in absence of this flux ($\mathbf{r} = 0$), the surface energy is decreasing (strictly for a nonstationary surface) and the total mass of the film is conserved.

We finally take a look on the structure of the adatom surface diffusion model, which can be seen well from (1.7), (1.8). The two equations can be interpreted as diffusion equations for the adatom density δ and the film height u , where the equation for δ includes *cross-diffusion* terms, i.e., second spatial derivatives of u .

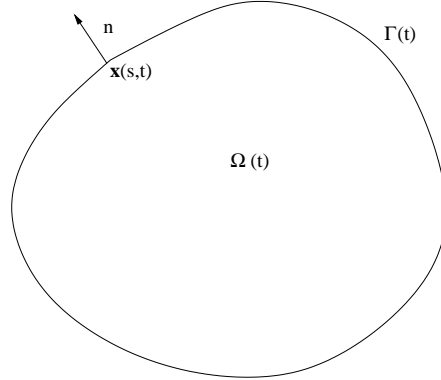


FIG. 2.2. Geometric setup in the case of a crystal growing by adatom surface diffusion.

2.3. Crystal growth. In the case of a crystal (as which we actually denote any closed curve or surface), we represent the bulk by a domain $\Omega(t) \subset \mathbb{R}^{d+1}$, $d = 1, 2$. The surface is then the whole boundary $\Gamma(t) = \partial\Omega(t)$ (see Figure 2.2).

The strong formulation of the adatom surface diffusion model is given by (1.7), (1.8). For the sake of brevity and simplicity we restrict the derivation of a weak formulation to the case $d=1$ and assume that the curve $\Gamma(t) = \partial\Omega(t)$ can be represented by an arclength parametrization of the form

$$\Gamma(t) = \{ \mathbf{x}(s,t) \mid \left| \frac{\partial \mathbf{x}}{\partial s}(s,t) \right| = 1, s \in [0, \lambda(t)] \}.$$

The tangent is obtained as $\mathbf{t} = \frac{\partial \mathbf{x}}{\partial s}$ and we use the orientation $\mathbf{n} = \left(\frac{\partial x_2}{\partial s}, -\frac{\partial x_1}{\partial s} \right)$ for the unit normal. In addition to the mean curvature we can introduce the curvature vector $\mathbf{K} = \kappa \mathbf{n} = \frac{\partial^2 \mathbf{x}}{\partial s^2}$. For the total velocity we obtain $\mathbf{V} = \frac{\partial \mathbf{x}}{\partial t}$, the normal velocity is $V = \mathbf{V} \cdot \mathbf{n}$, and the tangential velocity $\mathbf{v} = \mathbf{V} - V\mathbf{n}$.

In order to obtain a weak formulation we follow the approach in [7, 32] for parametric surface diffusion introducing weak forms for the scalar and vectorial quantities for velocities and curvatures. This yields after obvious integrations by parts with respect to s :

$$\begin{aligned} \int_0^{\lambda(t)} \left(\frac{\partial \delta}{\partial t} \varphi - \mathbf{V} \cdot \frac{\partial \mathbf{x}}{\partial s} \frac{\partial \delta}{\partial s} + L \frac{\partial \mu}{\partial s} \frac{\partial \varphi}{\partial s} + (\rho - \delta \kappa) V \varphi - \mathbf{r} \cdot \mathbf{n} \varphi \right) ds &= 0 \\ \int_0^{\lambda(t)} (bV - \psi \kappa - (\rho - \delta \kappa) \mu) w ds &= 0 \\ \int_0^{\lambda(t)} (\kappa - \mathbf{K} \cdot \mathbf{n}) \xi ds &= 0 \\ \int_0^{\lambda(t)} (V - \mathbf{V} \cdot \mathbf{n}) \zeta ds &= 0 \\ \int_0^{\lambda(t)} \left(\mathbf{K} \cdot \Phi + \frac{\partial \mathbf{x}}{\partial s} \cdot \frac{\partial \Phi}{\partial s} \right) ds &= 0 \\ \int_0^{\lambda(t)} \left(\mathbf{V} \cdot \Psi - \frac{\partial \mathbf{x}}{\partial t} \cdot \Psi \right) ds &= 0 \end{aligned}$$

for all sufficiently smooth scalar test functions φ, w, ξ, ζ , and sufficiently smooth vectorial test functions Φ, Ψ .

Global mass conservation for the mass functional

$$m(\Gamma(t), \delta(t)) = \int_{\Omega(t)} \rho d\mathbf{x} + \int_{\Gamma(t)} \delta dS$$

and global energy dissipation for

$$E(\Gamma(t), \delta(t)) = \int_{\Gamma(t)} \psi(\delta) dS$$

can be concluded as in the derivation of the model, resulting in

$$\frac{d}{dt} m(\Gamma(t), \delta(t)) = \int_{\Gamma(t)} \mathbf{r} \cdot \mathbf{n} dS$$

and

$$\frac{d}{dt} E(\Gamma(t), \delta(t)) = - \int_{\Gamma(t)} (bV^2 + L |\nabla_S \mu|^2 - \mu \mathbf{r} \cdot \mathbf{n}) dS.$$

2.4. Importance of the kinetic term. In [26] it has been argued that including the kinetic term $b \neq 0$ into the model is of particular importance, since it makes the second equation parabolic and therefore might have a regularizing effect. A detailed investigation of the relation (1.8) in the case $b=0$ shows that absence of the kinetic term (but included adatom densities) may yield unphysical behaviour of the model, namely either negative densities or transition to a convex surface with infinite speed.

Suppose that the solution satisfies $\delta \geq 0$ and $\rho^{\text{ef}} \geq 0$ and that the surface free energy functional $\delta \mapsto \psi(\delta)$ is an increasing function with $\psi(\delta) \geq \psi(0) > 0$. Then we have that $\mu = \psi'(\delta) \geq 0$ and for $b=0$ the curvature satisfies due to (1.8)

$$\kappa = -\frac{\rho^{\text{ef}}}{\psi} \mu \leq 0.$$

Hence, the surface is always convex for positive time, which means that nonconvex parts of the initial surface are removed at infinite speed, which seems to be an effect that does not model the actual physics. For positive values of the kinetic coefficient, nonconvex parts of the surface will still be removed, but in finite time.

For a film, the absence of the kinetic term has even more severe consequences. Under the same assumptions on δ and ψ as above, with positive effective density ρ^{ef} defined by (2.12), the height function satisfies

$$-\text{div} \left(\psi \frac{\nabla u}{Q} \right) = \rho^{\text{ef}} \mu \geq 0.$$

Hence, u is the solution of an elliptic partial differential equation of second order for arbitrary fixed t (note that the coefficient $\frac{\psi}{Q}$ is positive) and consequently, it cannot attain a strict minimum inside D . The only periodic function that does not attain a strict minimum inside the domain is a spatially constant one. Hence, the surface would transform to a flat film immediately, another unphysical effect happening since the kinetic term is ignored.

We finally mention that a similar argument could be applied to the original surface diffusion model (1.1), (1.2). However, in this case we would only obtain negativity of the chemical potential μ , which is not an unphysical effect at the first glance since μ is not related directly to a material density in (1.1), (1.2). However, as we shall see below, the original surface diffusion model (with additional kinetic term) can be derived formally as an asymptotic limit of (1.7), (1.8) for small adatom densities. In this asymptotic, μ corresponds to the limit of $\psi''(0)\delta$ and since we assume the free energy functional to be convex (i.e., $\psi'' \geq 0$), the chemical potential should be nonnegative, too. This argument might motivate a different future treatment of the model (1.1), (1.2), either via including a kinetic term or by deriving a modified limit of (1.7), (1.8).

2.5. Relation to known interface motion laws. In order to understand the relation to the frequently used models for the motion of interfaces, we compare the initial dynamics of the adatom surface diffusion model with the model of kinetic surface diffusion (also called *intermediate surface motion laws* in [24]), by which we understand (1.1), (1.2) with an additional kinetic term, i.e.,

$$-\text{div}_S(L\nabla_S \mu) + \rho V = \mathbf{r} \cdot \mathbf{n} \tag{2.15}$$

$$bV - \psi_0 \kappa - \rho \mu = 0. \tag{2.16}$$

Assume we are given the same initial surface and initial chemical potential and denote by V^{ASD} the velocity obtained from the adatom surface diffusion model and by V^{KSD} the velocity obtained from kinetic surface diffusion. Then, at time $t=0$ we have

$$b(V^{ASD} - V^{KSD}) = (\psi - \psi_0 - \delta\mu)\kappa.$$

Due to the convexity of ψ , we obtain $\psi(\delta) - \delta\mu \leq \psi_0$ and hence,

$$\begin{aligned} V^{ASD} &< V^{KSD} && \text{if } \kappa > 0 \\ V^{ASD} &> V^{KSD} && \text{if } \kappa < 0, \end{aligned}$$

i.e., the initial evolution by adatom surface diffusion is faster on concave and slower on convex parts of the surface. For the later evolution we cannot provide any rigorous arguments, but we expect a similar behaviour. In particular, the inclusion of adatoms into the model breaks the symmetry between convex and concave parts in general.

Another important relation to kinetic surface diffusion is a limiting behaviour as the cost of free adatoms tends to infinity. We shall illustrate this situation by a formal asymptotic expansion in a cost parameter β tending to infinity, assuming that the free energy is of the form $\psi(\delta) = \psi_0 + \beta\psi_1(\delta)$ with strictly convex $\psi_1: \mathbb{R} \rightarrow \mathbb{R}_+$ satisfying $\psi_1(0) = 0$. We then assume an asymptotic expansion of the adatom density in the form

$$\delta = \delta^0 + \beta^{-1}\delta^1 + \beta^{-2}\delta^2 + \mathcal{O}(\beta^{-3})$$

and of the surface as

$$\Gamma = \{\mathbf{x}^0(S) + \beta^{-1}\mathbf{x}^1(S) + \mathcal{O}(\beta^{-2})\}$$

with S being an appropriate surface parametrization. We assume that the expansion of the surface is sufficiently smooth in space and time, such that we can make an analogous expansion for the normal, curvature, and the normal velocity. As a consequence of the assumed form of the surface energy and the expansion of δ , we may expand the chemical potential as

$$\mu = \beta\psi_1'(\delta^0) + \psi_1''(\delta^0)\delta^1 + \mathcal{O}(\beta^{-1}).$$

Using these expansions in (1.7), (1.8), we obtain

$$\begin{aligned} -\beta(\operatorname{div}_S(L\nabla_S\psi_1'(\delta^0))) + Q_1 + \mathcal{O}(\beta) &= \mathbf{r} \cdot \mathbf{n}^0, \\ -\beta\psi_1(\delta^0)\kappa^0 - \beta(\rho - \delta^0\kappa^0)\psi_1'(\delta^0) + R_1 + \mathcal{O}(\beta) &= 0, \end{aligned}$$

where Q_1 and R_1 denote the zero order terms in the expansion (to be specified below). From the highest order term in the first equation we deduce that $\psi_1'(\delta^0)$ is constant over the surface, which implies that δ^0 is constant due to the strict monotonicity of ψ_1' . From the highest order term in the second equation we obtain

$$(\psi_1(\delta^0) - \delta^0\psi_1'(\delta^0))\kappa^0 = -\rho\psi_1'(\delta^0),$$

and hence, either $\psi_1'(\delta^0) = 0$ (which is equivalent to $\delta^0 = 0$) or κ^0 is a positive constant (a situation that is impossible e.g. in the film case). For $\delta^0 = 0$, the first-order terms in the expansion are given by

$$\begin{aligned} Q_1 &= -\operatorname{div}_S(L\nabla_S\mu^1) + \rho V^0 - \mathbf{r} \cdot \mathbf{n}^0 \\ R_1 &= bV^0 - \psi_0\kappa^0 - \rho\mu^1 \end{aligned}$$

with $\mu^1 = \psi_1''(\delta^0)\delta^1$. Hence, the first order asymptotic expansion of the adatom surface diffusion model, determined by $Q_1 = R_1 = 0$ is exactly the kinetic surface diffusion model (2.15), (2.16).

The kinetic surface diffusion model is clearly not the only one we can obtain as a limit. If, in addition to the assumptions above, we have a small kinetic coefficient expanded as

$$b = b_0\beta^{-1} + \mathcal{O}(\beta^{-2}),$$

then the lowest order expansion as well as the term Q_1 remain the same, but $R_1 = -\psi_0\kappa^0 - \rho\mu^1$. Hence, the asymptotic limit in this situation is given by the surface diffusion law (1.1),(1.2). However, as we noticed already before the formal expansion might not be correct if $\kappa^0 > 0$ since without additional correction terms the limiting chemical potential μ^1 would become negative abruptly. A detailed analysis and further understanding of this effect remains an important challenge for future investigations of surface diffusion.

An interesting dynamic of a different type appears as a limit when the kinetic coefficient $b > 0$ is fixed and the mobility of the adatoms is large, i.e., $L = L_0\beta + L_1 + \mathcal{O}(\beta^{-1})$. In this case, with the same expansion of δ and V as above, we obtain

$$\begin{aligned} & -\beta^2 \operatorname{div}_S(L_0\nabla_S\psi_1'(\delta^0)) - \beta \operatorname{div}_S(L_1\nabla_S\psi_1'(\delta^0)) \\ & \quad - \beta \operatorname{div}_S(L_0\nabla_S\psi_1''(\delta^0)\delta^1) + Q_1 + \mathcal{O}(\beta) = \mathbf{r} \cdot \mathbf{n}^0 \\ & -\beta\psi_1(\delta^0)\kappa^0 - \beta(\rho - \delta^0\kappa^0)\psi_1'(\delta^0) + R_1 + \mathcal{O}(\beta) = 0. \end{aligned}$$

The treatment of the lowest order terms is the same as above, and in particular for the film case $\delta^0 = 0$ is the only possible solution. As a consequence, the first order term in the first equation implies $\operatorname{div}_S(L_0\nabla_S\psi_1''(0)\delta^1) = 0$ and hence, δ^1 is constant with respect to S . The terms to vanish at the next order are given by

$$\begin{aligned} Q_1 &= -\operatorname{div}_S(L\nabla_S\psi_1'''(0)\delta^2) + \rho V^0 - \mathbf{r} \cdot \mathbf{n}^0 \\ R_1 &= bV^0 - \psi_0\kappa^0 - \rho\psi_1''(0)\delta^1. \end{aligned}$$

From $Q_1 = 0$ we deduce

$$0 = \int_{\Gamma(t)} Q_1 \, dS = \int_{\Gamma(t)} (\rho V^0 - \mathbf{r} \cdot \mathbf{n}^0) \, dS,$$

i.e., a formula for the mean value of the velocity. Moreover we derive from $R_1 = 0$ that

$$\begin{aligned} 0 &= \int_{\Gamma(t)} R_1 \, dS = \int_{\Gamma(t)} (bV^0 - \psi_0\kappa^0 - \rho\psi_1''(0)\delta^1) \, dS \\ &= \frac{b}{\rho} \int_{\Gamma(t)} \mathbf{r} \cdot \mathbf{n}^0 \, dS - \psi_0 \int_{\Gamma(t)} \kappa^0 \, ds - |\Gamma(t)|\rho\psi_1''(0)\delta^1. \end{aligned}$$

We can insert the last relation again into $R_1 = 0$ and derive as a limit

$$bV - \psi_0 \left(\kappa - \frac{1}{|\Gamma(t)|} \int_{\Gamma(t)} \kappa \, dS \right) = \frac{b}{\rho|\Gamma(t)|} \int_{\Gamma(t)} \mathbf{r} \cdot \mathbf{n}^0 \, dS, \quad (2.17)$$

a well-known model of surface attachment limited kinetics (SALK). In the absence of a deposition flux, this limit becomes the volume-conserving version of the mean-curvature flow

$$bV - \psi_0 \left(\kappa - \frac{1}{|\Gamma(t)|} \int_{\Gamma(t)} \kappa \, dS \right) = 0. \quad (2.18)$$

3. Equilibrium structures

In the following we consider equilibrium structures of surfaces with free adatoms. We distinguish between *local equilibria* determined as stationary solutions of (1.7), (1.8), and *global equilibria*, obtained as the global minimizers of the surface energy subject to a mass constraint. We start by discussing the properties of the surface energy.

3.1. Surface energy. In the following we further investigate the structure of the surface energy term in the presence of adatom densities. For the sake of simplicity we restrict most arguments to the film case. The surface energy for a film is given by

$$\hat{E}(\delta, u) := E(\Gamma, \delta) = \int_D \psi(\delta) Q \, d\mathbf{x}. \quad (3.1)$$

Throughout the remainder of the paper we make the following assumption on the surface free energy ψ :

ASSUMPTION 3.1. *We assume that $\psi: \mathbb{R} \rightarrow \mathbb{R}_+$ is twice continuously differentiable and strictly convex. Moreover, we assume that ψ attains its unique minimum at 0, with $\psi(0) = 1 > 0$.*

In several cases below we will also consider a prototype free energy of the form

$$\psi(\delta) = 1 + \frac{\gamma}{2} \delta^2. \quad (3.2)$$

Under Assumption 3.1, the functional $\delta \mapsto \psi(\delta) - 1$ is nonnegative and strictly convex and we have $Q \geq 1$. Hence, for δ and u sufficiently smooth, there exists a constant $c > 0$ such that

$$\hat{E}(\delta, u) = \int_D ((\psi(\delta) - 1) Q + Q) \, d\mathbf{x} \geq c \int_D \delta^2 \, d\mathbf{x} + \int_D |\nabla u| \, d\mathbf{x}.$$

This argument shows that the energy functional uniformly bounds the L^2 -norm of δ and the total variation of u . Hence, it is natural to consider the energy minimization in the spaces $L^2(D)$ (for δ) and a space of functions of bounded variation (for u). Unfortunately, the energy functional is unbounded in these spaces, so that we have to expect ill-posedness of the adatom surface diffusion model for general data. As we shall see below, the surface energy is not convex (even in stronger topologies), but at least global minimizers of the energy at constant mass can be computed.

3.2. Non-convexity of the surface energy. In the following we investigate the properties of the surface energy functional \hat{E} . We start by computing the first and second derivatives:

LEMMA 3.1. *The surface energy functional \hat{E} defined via (3.1) is twice Fréchet-differentiable on $L^\infty(D) \times W^{1,\infty}(D)$ with derivatives given by*

$$\hat{E}'(\delta, u)(\eta, v) = \int_D \left(\mu(\delta) \eta Q + \psi(\delta) \frac{\nabla u \cdot \nabla v}{Q} \right) d\mathbf{x}$$

for all $\eta \in L^\infty(D)$ and all $v \in W^{1,\infty}(D)$, and

$$\begin{aligned} \hat{E}''(\delta, u)(\eta_1, v_1; \eta_2, v_2) &= \int_D \left(\psi''(\delta) \eta_1 \eta_2 Q + \psi(\delta) \frac{(\mathbf{P} \nabla v_1) \cdot \nabla v_2}{Q^3} \right) d\mathbf{x} \\ &+ \int_D \left(\mu(\delta) \eta_1 \frac{\nabla u \cdot \nabla v_2}{Q} + \mu(\delta) \eta_2 \frac{\nabla u \cdot \nabla v_1}{Q} \right) d\mathbf{x} \end{aligned}$$

for all $\eta_1, \eta_2 \in L^\infty(D)$ and all $v_1, v_2 \in W^{1,\infty}(D)$.

In order to obtain information about the convexity of the surface energy we investigate the coercivity properties of the second derivative at different points. It turns out that for surfaces close enough to flat surfaces, $\hat{E}''(\delta, u)$ is positive definite:

THEOREM 3.1. *For each $\delta \in L^\infty(D)$ there exist constants $c_1, c_2 \in \mathbb{R}^+$ such that*

$$\hat{E}''(\delta, u)(\eta, v; \eta, v) \geq c_1 \int_D (\eta^2 + |\nabla v|^2) \, d\mathbf{x} \quad (3.3)$$

for all $u \in W^{1,\infty}(D)$ such that $|\nabla u| \leq c_2$ almost everywhere in D .

Proof. Since ψ is strictly convex, we have

$$c := \inf_{\delta} \psi''(\delta) > 0.$$

Using the Cauchy-Schwarz and arithmetic-geometric-mean inequalities we can estimate the surface energy as

$$\begin{aligned} \hat{E}''(\delta, u)(\eta, v; \eta, v) &\geq \int_D \left(c\eta^2 Q + \psi(\delta) \frac{(\mathbf{P}\nabla v) \cdot \nabla v}{Q^3} \right) \, d\mathbf{x} \\ &\quad - \int_D \left((1-\epsilon)c\eta^2 Q + \frac{\mu(\delta)^2}{c(1-\epsilon)} \frac{|\nabla u \cdot \nabla v|^2}{Q^3} \right) \, d\mathbf{x} \end{aligned}$$

for each $\epsilon \in (0, 1)$. Since $Q \geq 1$ and

$$(\mathbf{P}\nabla v) \cdot \nabla v = Q^2 |\nabla v|^2 - |\nabla u \cdot \nabla v|^2,$$

we may conclude for $|\nabla u| \geq c_2$

$$\hat{E}''(\delta, u)(\eta, v; \eta, v) \geq \int_D \left(\epsilon c\eta^2 + (\psi(\delta)(1-c_2^2) - \frac{c_2^2 \mu(\delta)^2}{c(1-\epsilon)}) \frac{|\nabla v|^2}{Q} \right) \, d\mathbf{x}.$$

Since all terms depending on δ and Q are bounded in $L^\infty(D)$, we can choose ϵ , c_1 and c_2 sufficiently small such that (3.3) is satisfied. \square

For positive adatom density and a very rough surface ($|\nabla u|$ large), the contrary to the above statement is true, i.e., we can find a direction in which the second derivative is negative:

THEOREM 3.2. *Let $\delta \in L^\infty(D)$ be such that $\delta \geq \delta_0$ almost everywhere for some constant $\delta_0 \in \mathbb{R}_+$. Then, for each $u \in W^{1,\infty}(D)$ satisfying $|\nabla u| \geq c_0$ almost everywhere for a sufficiently large constant $c_0 \in \mathbb{R}_+$, there exists a pair $(\eta, v) \in L^\infty(D) \times W^{1,\infty}(D)$ such that*

$$\hat{E}''(\delta, u)(\eta, v; \eta, v) < 0.$$

Proof. Let

$$C := \sup_{\mathbf{x} \in D} \psi''(\delta), \quad c := \inf_{\mathbf{x} \in D} \psi''(\delta)$$

and $\lambda := \frac{C}{c} + 1$ (note that c and C are finite, and due to the strict convexity of ψ , c is positive). Because of $\psi(0) = 1$ and $\psi'(0) = 0$ we can estimate $c\delta \leq \psi'(\delta) \leq C\delta$ and $\psi(\delta) \leq 1 + \frac{C}{2}\delta^2$ almost everywhere.

We now choose $\eta = -\delta$ and $v = \lambda u$. Then, we have the following estimates for the terms appearing in the second derivative (in the almost everywhere sense):

$$\begin{aligned}\psi''(\delta)\eta^2Q &= \frac{\psi''(\delta)\delta^2}{Q}(1+|\nabla u|^2) \leq \frac{C\delta^2}{Q}(1+|\nabla u|^2) \\ \psi(\delta)\frac{(\mathbf{P}\nabla v)\cdot\nabla v}{Q^3} &= \lambda^2\psi(\delta)\frac{|\nabla u|^2}{Q^3} \leq \lambda^2\left(1+\frac{C\delta^2}{2}\right)\frac{|\nabla u|^2}{Q^3} \\ 2\psi'(\delta)\eta\frac{\nabla u\cdot\nabla v}{Q} &= -2\lambda\psi'(\delta)\delta\frac{|\nabla u|^2}{Q} \leq -2\lambda c\delta^2\frac{|\nabla u|^2}{Q}.\end{aligned}$$

From the definition of λ we obtain

$$\frac{C\delta^2}{Q}(1+|\nabla u|^2) - \lambda c\delta^2\frac{|\nabla u|^2}{Q} = \frac{\delta^2}{Q}(C - c|\nabla u|^2) \leq \frac{\delta_0^2}{Q}(C - cc_0^2) < 0$$

for $c_0 > \sqrt{\frac{C}{c}}$. Moreover, for $c_0^2 > \lambda\frac{C}{2c} - 1$ we have

$$\begin{aligned}\lambda^2\left(1+\frac{C\delta^2}{2}\right)\frac{|\nabla u|^2}{Q^3} - \lambda c\delta^2\frac{|\nabla u|^2}{Q} &= \lambda\frac{|\nabla u|^2}{Q^3}\left(\lambda+\frac{C\delta^2}{2}\lambda - c\delta^2Q^2\right) \\ &\leq \lambda\frac{|\nabla u|^2}{Q^3}\left(\lambda - \delta_0^2\left(c+cc_0^2 - \lambda\frac{C}{2}\right)\right)\end{aligned}$$

and the last term is negative for $c_0^2 > \lambda\frac{(2+C\delta_0^2)}{2c\delta_0^2}$. Hence, for c_0 sufficiently large, we obtain

$$I(\eta, v) := \psi''(\delta)\eta^2Q + \psi(\delta)\frac{(\mathbf{P}\nabla v)\cdot\nabla v}{Q^3} + 2\psi'(\delta)\eta\frac{\nabla u\cdot\nabla v}{Q} < 0$$

almost everywhere, and consequently

$$\hat{E}''(\delta, u)(\eta, v; \eta, v) = \int_D I(\eta, v) \, d\mathbf{x} < 0.$$

□

From the motivation of the model it seems obvious that undesirable effects like nonconvex energies can occur for large adatom densities. Note however that as a consequence of Theorem 3.2, the surface energy cannot be globally convex for positive adatom density (even arbitrarily small) and very rough surfaces.

3.3. Equilibrium films. The global equilibrium film structure at given mass is determined as a global minimizer of

$$\hat{E}(\delta, u) \rightarrow \min_{\delta, u} \quad \text{subject to } \hat{m}(\delta, u) = m_0 \quad (3.4)$$

with the mass \hat{m} given by

$$\hat{m}(\delta, u) = \int_D (\rho u + \delta Q) \, d\mathbf{x}. \quad (3.5)$$

As one can see from the discussion in the previous section, we cannot conclude the existence of a minimizer by standard arguments such as lower semicontinuity of the

energy functional and compactness of its level sets. However, we can explicitly compute the global energy minimizer, determined by a flat surface and vanishing adatom density.

THEOREM 3.3. *The variational problem (3.4) has a unique global minimizer in $L^\infty_{per}(D) \times W^{1,\infty}_{per}(D)$, given by*

$$(\hat{\delta}(\mathbf{x}), \hat{u}(\mathbf{x})) = \left(0, \frac{m_0}{\rho|D|}\right), \quad \forall \mathbf{x} \in D.$$

Moreover, $(\hat{\delta}, \hat{u})$ is the unique stationary point of \hat{E} subject to constrained mass \hat{m} .

Proof. We have

$$\hat{E}(\hat{\delta}, \hat{u}) = \int_D \psi(0) \, d\mathbf{x} = |D|.$$

Since $\psi(0)=1$ is the unique global minimum of ψ and $Q \geq 1$ (with identity only if $\nabla u = 0$), we conclude that

$$\hat{E}(\delta, u) = \int_D \psi(\delta) Q \, d\mathbf{x} \geq \int_D 1 \, d\mathbf{x},$$

with equality if and only if $\nabla u \equiv 0$ and $\delta \equiv 0$. Since the only pair (δ, u) satisfying these properties as well as the mass constraint is given by $(\hat{\delta}, \hat{u})$, this pair is a unique global minimizer of (3.4) subject to (3.5).

We now turn our attention to stationary points, i.e., weak solutions of (2.13), (2.14) with $\frac{\partial \delta}{\partial t} = 0$, $\frac{\partial u}{\partial t} = 0$, and $\mathbf{r} = 0$. From (2.13) we observe that each local equilibrium satisfies

$$\int_D L \frac{\mathbf{P} \nabla \mu \cdot \nabla \varphi}{Q} \, d\mathbf{x} = 0,$$

for all sufficiently smooth tests of functions φ . Due to the positive definiteness of the coefficient matrix $L \frac{\mathbf{P}}{Q}$ we obtain that μ is constant, which implies with the strict monotonicity of ψ' that δ is constant. Using these results in (2.14) we further deduce

$$(\psi - \delta \mu) \int_D \frac{\nabla u \cdot \nabla w}{Q} \, d\mathbf{x} = \rho \mu \int_D w \, d\mathbf{x}.$$

for all sufficiently smooth test function w . Using the particular constant function $w \equiv 1$, we obtain that $\mu = 0$, and hence,

$$\psi \int_D \frac{\nabla u \cdot \nabla w}{Q} \, d\mathbf{x} = 0,$$

for all w , which implies that u is constant. Since ψ is a convex function with unique minimum at $\delta = 0$, $\mu = \psi'(\delta) = 0$ is only possible for $\delta = 0$. Thus, from the mass constraint we obtain that $(\hat{\delta}, \hat{u})$ as above is also the unique stationary point. \square

3.4. Equilibrium crystals. In the crystal case, the global equilibrium is determined by the minimization of the surface energy E (defined via (1.12)) subject to a mass constraint, i.e.,

$$E(\Gamma, \delta) \rightarrow \min_{\Gamma = \partial\Omega, \delta} \quad \text{subject to } m(\Gamma, \delta) = m_0. \quad (3.6)$$

In the absence of free adatoms, the minimization of the surface energy is a famous problem, whose solution, i.e., the minimizer of

$$E(\Gamma, 0) \rightarrow \min_{\Gamma=\partial\Omega} \quad \text{subject to } m(\Gamma, 0) = m_0. \quad (3.7)$$

is called the *Wulff shape*. In the isotropic case, it is well-known due to isoperimetric inequalities that the Wulff shape Γ_W is a sphere, with radius determined by the mass constraint as $R_W = \left(\frac{m_0}{\rho\omega_d}\right)^{1/(d+1)}$, where ω_d denotes the volume of the unit ball in \mathbb{R}^{d+1} . Surprisingly, and opposed to the film case discussed above, this property is not true in the crystal case, as a consequence of the following result:

PROPOSITION 3.4. *Let Γ_W be the sphere with radius $R_W = \left(\frac{m_0}{\rho\omega_d}\right)^{1/(d+1)}$. Then, there exists $\epsilon > 0$ such that for $R \in (R_W - \epsilon, R_W)$ and Γ_R being the sphere with radius R ,*

$$E(\Gamma_R, \delta_R) < E(\Gamma_W, 0),$$

where δ_R is the constant positive adatom density determined via $m(\Gamma, \delta_R) = m_0$, i.e.,

$$\delta_R = \frac{m_0 - \rho\omega_d R^{d+1}}{\sigma_d R^d},$$

with σ_d being the surface area of the unit sphere in \mathbb{R}^{d+1} .

Proof. From the above formula for δ_R we conclude that δ_R is continuously differentiable with respect to R and the derivative is given by

$$\frac{d\delta_R}{dR} = - \left(\frac{dm_0}{\sigma_d R^{d+1}} + \frac{\rho\omega_d}{\sigma_d} \right) < 0.$$

We consider the function

$$e(R) := E(\Gamma_R, \delta_R) = \sigma_d \psi(\delta_R) R^d,$$

which is then also continuously differentiable with derivative

$$\frac{de}{dR}(R) = d\sigma_d \psi(\delta_R) R^{d-1} + \sigma_d \psi'(\delta_R) R^d \frac{d\delta_R}{dR}.$$

At $R = R_W$ we have $\delta_R = 0$ and since ψ has a minimum at 0, we have $\psi'(\delta_R) = 0$. Thus, $\frac{de}{dR}(R) = d\sigma_d R_W^{d-1} > 0$, which implies the assertion due to the continuous differentiability of e . \square

Proposition 3.4 shows that the Wulff shape with vanishing adatom density cannot be a global minimizer of the energy, it cannot even be a local equilibrium (it is a strict local maximum in the class of radially symmetric shapes and constant adatom densities). We shall now show that the global equilibrium is still attained at constant adatom density and a spherical shape:

THEOREM 3.5. *The global minimizer of the surface energy at constant mass is attained for some shape Γ_R being the minimizer among all spheres with radius $R < R_W$ at a constant adatom density $\delta_R = \frac{m_0 - \rho\omega_d R^{d+1}}{\sigma_d R^d}$. For each stationary point $(\hat{\Gamma}, \hat{\delta})$, i.e. a solution of (1.7), (1.8) with $\frac{\partial \delta}{\partial t} \equiv 0$ and $V \equiv 0$, the adatom density $\hat{\delta}$ and the mean curvature κ of $\hat{\Gamma}$ are constant.*

Proof. Let $\Gamma = \partial\Omega$, let $\Gamma_0 \subset \Gamma$, and let δ be an arbitrary nonnegative function on Γ . Then we define

$$\hat{\delta} = \begin{cases} \delta & \text{on } \Gamma \setminus \Gamma_0 \\ \frac{1}{|\Gamma_0|} \int_{\Gamma_0} \delta \, dS & \text{on } \Gamma_0. \end{cases}$$

From the construction we see $m(\Gamma, \delta) = m(\Gamma, \hat{\delta})$, and, because of the convexity of ψ ,

$$\begin{aligned} E(\Gamma, \hat{\delta}) - E(\Gamma, \delta) &= \int_{\Gamma_0} (\psi(\hat{\delta}) - \psi(\delta)) \, dS \leq \int_{\Gamma_0} \psi'(\hat{\delta})(\hat{\delta} - \delta) \, dS \\ &= \psi'(\hat{\delta}|_{\Gamma_0}) \int_{\Gamma_0} (\hat{\delta} - \delta) \, dS = 0, \end{aligned}$$

where we have used the fact that $\hat{\delta}$ is constant on Γ_0 and has the same mean value as δ . Hence, at fixed shape the energy can always be decreased locally by averaging, which implies that no state with nonconstant adatom density can be stable. In particular, we may conclude that there exists a global minimizer with constant adatom density. The fact that the minimizer for constant adatom density is of spherical shape follows from the isoperimetric inequality and since we have shown above that the Wulff shape is not an equilibrium, the radius of the equilibrium shape is smaller than R_W .

For a stationary solution (1.7), (1.8) we have $\operatorname{div}_S(L\nabla_S\hat{\delta}) = 0$, which implies that $\hat{\delta}$ is constant due to the closedness of the surface. Consequently, $\psi(\hat{\delta})$ and the corresponding chemical potential $\mu = \psi'(\hat{\delta})$ are constant, too. Equation (1.8) then reduces to $\kappa = \frac{\hat{\delta}\mu}{\psi(\hat{\delta}) - \delta\mu}$, which implies that the mean curvature is constant. \square

We mention that the stationary points depend on the spatial dimension. For curves ($d=1$) a stationary point is a circle, while for $d \geq 2$ also different surfaces with constant mean curvature can be found, which are all stationary points.

In order to gain insight into the behaviour of the minimizer with respect to the surface free energy, we consider a special example using the prototype surface free energy (3.2).

EXAMPLE 3.6. We consider the special case of a two-dimensional crystal ($d=1$) with the surface free energy ψ given by (3.2). In this case the only stationary point is a radially symmetric equilibrium shape with radius R and constant adatom density δ_R , satisfying

$$\delta_R = \frac{m_0 - \rho R^2 \pi}{2R\pi}$$

due to the mass constraint.

In order to obtain the minimizer of (3.6) over the special class of radially symmetric shapes and constant adatom densities, we can equivalently consider the minimization of the functional

$$e(R) := E(B_R, \delta_R) = R\pi(2 + \gamma\delta_R^2) = R\pi\left(2 + \gamma \frac{(m_0 - \rho R^2 \pi)^2}{(2R\pi)^2}\right)$$

with respect to $R \in (0, R_W]$. Plots of the energy functional e for different values of γ are shown in Figure 3.1 (for $\rho = 1$). We have seen above that the Wulff shape $R = R_W$

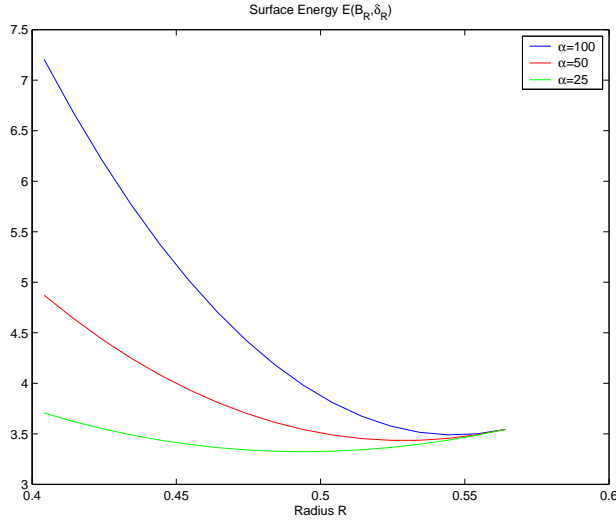


FIG. 3.1. Plot of the surface energy $E(B_R, \delta_R)$ in Example 3.6, with constant adatom density $\delta_R = \frac{m - \rho R^2 \pi}{2R\pi}$.

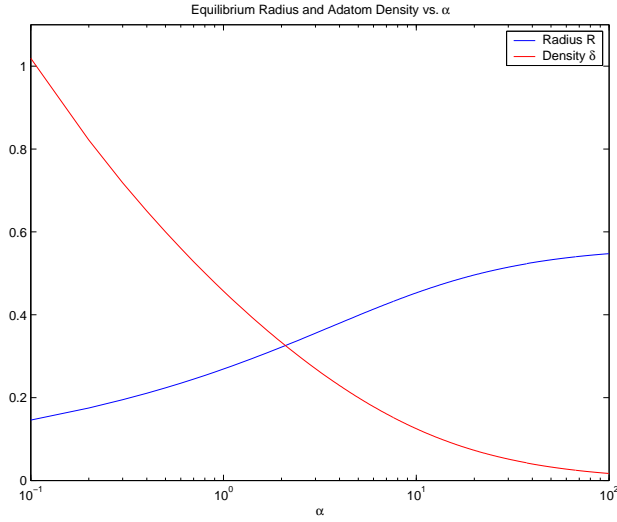


FIG. 3.2. Equilibrium values of the radius R and the adatom density δ_R for different values of γ in (3.2).

is not a minimizer and hence, we look for a minimizer R_* in the interior, which must satisfy

$$0 = \frac{de}{dR}(R_*) = 2\pi + \frac{\gamma}{4R_*^2\pi}(m_0 - \rho R_*^2\pi)(m_0 + 3\rho R_*^2\pi).$$

This yields a fourth order algebraic equation for the radius R_* , having two imaginary solutions: one negative real and one positive real. Since we are only interested in

positive real solutions, the unique stationary point in the interval $(0, R_W)$ is given by

$$R_* = \frac{1}{\sqrt{3\rho}} \sqrt{\frac{m_0}{\pi} - \frac{4}{\gamma} + \sqrt{\left(\frac{m_0}{\pi} - \frac{4}{\gamma}\right)^2 + \frac{3m_0^2}{\pi^2}}}.$$

One observes that for $\gamma \rightarrow \infty$, the equilibrium radius tends to the radius $R_W = \sqrt{\frac{m_0}{\rho\pi}}$ of the Wulff shape. On the other hand, for $\gamma \rightarrow 0$, the equilibrium radius tends to zero. This behaviour is not surprising, since the parameter γ measures the energetic cost of free adatoms. If γ is large, it is not energetically favourable to have free adatoms, while for γ small the energy can be decreased by releasing adatoms. However, if γ is very small and thus $R_* \ll R_W$, the continuum model probably does not correctly represent the physics, since there are more free adatoms than atoms in the bulk. A plot of the equilibrium radius R_* and the corresponding adatom density δ_{R_*} vs. the value of γ is shown in Figure 3.2.

4. Special dynamics

In this section we study the dynamics of adatom surface diffusion in special situations, in particular for small adatom densities.

4.1. Almost flat films. In the following we study the dynamics of (2.9), (2.10) around a flat surface with an adatom density being almost spatially homogeneous. For the sake of simplicity we consider a deposition flux being homogeneous in the vertical direction, i.e., $r_3 = r_3(t)$ and that $\mathbf{r}_{12} = 0$. We assume that the initial values satisfy

$$\delta_0(\mathbf{x}) = \delta_0^0 + \epsilon \delta_0^1(\mathbf{x}) + \mathcal{O}(\epsilon^2), \quad (4.1)$$

$$u_0(\mathbf{x}) = u_0^0 + \epsilon u_0^1(\mathbf{x}) + \mathcal{O}(\epsilon^2), \quad (4.2)$$

and look for solutions of (2.9), (2.10) in an expansion of the form

$$\delta(\mathbf{x}, t) = \delta^0(t) + \epsilon \delta^1(\mathbf{x}, t) + \mathcal{O}(\epsilon^2), \quad (4.3)$$

$$u(\mathbf{x}, t) = u^0(t) + \epsilon u^1(\mathbf{x}, t) + \mathcal{O}(\epsilon^2). \quad (4.4)$$

Then we can also expand the chemical potential in terms of δ^0 and δ^1 as

$$\mu(\mathbf{x}, t) = \psi'(\delta^0(t)) + \epsilon \frac{d^2\psi}{d\delta^2}(\delta^0(t)) \delta^1(\mathbf{x}, t) + \mathcal{O}(\epsilon^2).$$

Since we can assume that all mass and the mean height are included in δ_0^0 and u_0^0 , respectively, we can restrict our attention to perturbations satisfying

$$\int_D \delta_0^1 d\mathbf{x} = \int_D u_0^1 d\mathbf{x} = 0.$$

We shall verify below that the property of mean zero is conserved also for u^1 and δ^1 at later time $t > 0$.

Lowest order expansion. The zero-order expansion of (2.9), (2.10) is obtained as the solution of the a system of ordinary differential equations characterizing the spatially homogeneous situation:

$$\frac{d}{dt}(\delta^0 + \rho u^0) = r_3 \quad (4.5)$$

$$b \frac{du^0}{dt} - \rho \psi'(\delta^0) = 0, \quad (4.6)$$

with initial values u_0^0 and δ_0^0 . Note that (4.5) corresponds to the conservation of the total mass $m = (\delta^0 + \rho u^0)|D|$, and (4.6) can be interpreted as the energy dissipation relation at zero order.

We collect some results on (4.5), (4.6) in the following:

THEOREM 4.1. *For all initial values $(\delta_0^0, u_0^0) \in \mathbb{R}_+^2$ and each $r_3 \in C([0, T])$, there exists a unique solution $(\delta^0, u^0) \in C^1([0, T])^2$ of (4.5), (4.6). If the initial values are nonnegative, then $(\delta^0(t), u^0(t)) \geq (0, u_0^0)$ for all $t \in [0, t]$. Moreover, in the absence of deposition ($r_3 = 0$) $\delta^0(t)$ decays to zero exponentially, more precisely*

$$\delta^0(t) \leq e^{-cb^{-1}\rho^2 t/2},$$

where $c = \inf_{\delta} \psi''(\delta) > 0$.

Proof. Existence and uniqueness follows from the Picard-Lindelöf Theorem for ordinary differential equations. We can eliminate $\frac{du^0}{dt}$ to obtain the first-order equation

$$\frac{d\delta^0}{dt} + b^{-1}\rho^2\psi'(\delta^0) = r_3. \quad (4.7)$$

Standard arguments for ordinary differential equations imply that $\delta^0 \geq 0$ if $\delta_0^0 \geq 0$ and $r_3 \geq 0$. For the film height we obtain

$$\rho \frac{du^0}{dt} = r_3 - \frac{d\delta^0}{dt} = b^{-1}\rho^2\psi'(\delta^0) \geq 0,$$

i.e., monotone growth, which is stopped only when there are no free adatoms ($\delta^0 = 0$).

Moreover, we have

$$\psi'(\delta^0)\delta^0 = \psi(\delta^0) - \psi(0) + \frac{1}{2}(\delta^0)^2 \int_0^1 \frac{d^2\psi}{d\delta^2}(\sigma\delta^0) d\sigma \geq \frac{c}{2}(\delta^0)^2.$$

Hence, by multiplying (4.7) with $2\delta^0$ we obtain

$$\frac{d}{dt}(\delta^0)^2 + cb^{-1}\rho^2(\delta^0)^2 \leq 2r_3\delta_0.$$

For $r_3 = 0$ this estimate implies the exponential decay. \square

We finally mention that in the presence of a deposition flux, we may conclude that $\delta^0(t)$ decreases if $cb^{-1}\rho^2\delta^0 > 2r_3$, i.e., the adatom density is not too small and the deposition is not too fast.

First order expansion. We now proceed to the first-order expansion of (2.9), (2.10), which determines the evolution of spatial heterogeneities. We start with an expansion of the length of a surface element $Q = \sqrt{1 + |\nabla u|^2}$, which we obtain as

$$Q = 1 + \epsilon \frac{\nabla u^0 \cdot \nabla u^1}{Q} + \mathcal{O}(\epsilon^2),$$

and since $\nabla u^0 \equiv 0$, we conclude that the first-order expansion of Q vanishes. By analogous reasoning we obtain that the matrix \mathbf{P} is expanded as

$$\mathbf{P} = \mathbf{I} + \mathcal{O}(\epsilon^2).$$

Inserting these relations we derive the system

$$\frac{\partial \delta^1}{\partial t} - Lc_0 \Delta \delta^1 - \frac{du^0}{dt} \delta^0 \Delta u^1 + \rho \frac{\partial u^1}{\partial t} = 0 \quad (4.8)$$

$$b \frac{\partial u^1}{\partial t} - (\psi(\delta^0) - \mu^0 \delta^0) \Delta u^1 - \rho c_0 \delta^1 = 0, \quad (4.9)$$

for (δ^1, u^1) , where $c_0 := \frac{\partial^2 \psi}{\partial \delta^2}(\delta^0)$. The mean values

$$m^1(t) := \int_D \delta^1(\mathbf{x}, t) \, d\mathbf{x}, \quad h^1(t) := \int_D u^1(\mathbf{x}, t) \, d\mathbf{x}$$

satisfy the system of ordinary differential equations

$$\frac{d}{dt}(m^1 + \rho h^1) = 0, \quad \frac{dh^1}{dt} = \rho c_0 m^1,$$

with homogeneous initial values $m^1(0) = h^1(0) = 0$. Thus, the unique solution is given by $m^1(t) = h^1(t) = 0$, i.e., the zero mean values are conserved in time.

We can insert the relations for $\frac{du^0}{dt}$ and $\frac{\partial u^1}{\partial t}$ into (4.8) to obtain

$$\frac{\partial \delta^1}{\partial t} - Lc_0 \Delta \delta^1 + b^{-1} \rho^2 c_0 \delta^1 + b^{-1} \rho (\psi(\delta^0) - 2\mu^0 \delta^0) \Delta u^1 = 0 \quad (4.10)$$

$$b \frac{\partial u^1}{\partial t} - (\psi(\delta^0) - \mu^0 \delta^0) \Delta u^1 - \rho c_0 \delta^1 = 0, \quad (4.11)$$

with the notation $\mu^0 = \psi'(\delta^0)$. In the form (4.10), (4.11) the cross-diffusion structure of the system can be seen very well, we obtain a cross-diffusion term in the parabolic equation for δ^1 .

Note that for the effective diffusion coefficient in (4.9) or (4.11) we obtain

$$\frac{d}{dt} (\psi(\delta^0) - \mu^0 \delta^0) = \mu^0 \frac{d\delta^0}{dt} - \mu^0 \frac{d\delta^0}{dt} - \frac{d\mu^0}{dt} \delta^0 = -\frac{d^2 \psi}{d\delta^2}(\delta^0) \frac{d\delta^0}{dt} \delta^0.$$

Inserting (4.7) we deduce

$$\frac{d}{dt} (\psi(\delta^0) - \mu^0 \delta^0) = \frac{d^2 \psi}{d\delta^2}(\delta^0) (b^{-1} \rho^2 \psi'(\delta^0) - r_3) \delta^0.$$

This term is nonnegative for $r_3 \leq b^{-1} \rho^2 \mu^0$, and in particular for $r_3 = 0$ the coefficient $\psi(\delta^0) - \mu^0 \delta^0$ is nondecreasing in time. Hence, if the initial value satisfies $\psi(\delta_0^0) - \mu_0^0 \delta_0^0 \geq a > 0$ for some $a \in \mathbb{R}$, then

$$\psi(\delta^0(t)) - \mu^0(t) \delta^0(t) > a, \quad \forall t \in [0, T]. \quad (4.12)$$

Because of the physical interpretation as a system with underlying energy dissipation, we do not look for standard weak solutions with $(\delta_0^1, u_0^1) \in L^2_{\text{per}}(D)^2$. As a motivation we consider a second-order expansion of the energy around the equilibrium $(\delta_0^0, u_0^0) = (0, \frac{m}{\rho|D|})$, which is given by

$$\int_D \psi(\delta_0) \sqrt{1 + |\nabla u_0|^2} \, d\mathbf{x} = |D| + \frac{\epsilon^2}{2} \int_D (\psi''(0) (\delta_0^0)^2 + |\nabla u_0^1|^2) + \mathcal{O}(\epsilon^3).$$

Hence, in order to guarantee that the first non-trivial term in the energy expansion is defined, we have to look for weak solutions corresponding to initial values

$$(\delta_0^1, u_0^1) = L_{\text{per}}^2(D) \times H_{\text{per}}^1(D).$$

We denote the product space for the weak solution as

$$\begin{aligned} \mathcal{V}_{\text{per}} := & \{(\delta^1, u^1) \mid \delta^1 \in C(0, T; H_{\text{per}}^1(D)) \cap C([0, T]; L_{\text{per}}^2(D)) \\ & \cap C^1(0, T; H_{\text{per}}^{-1}(D)), u^1 \in C(0, T; H_{\text{per}}^2(D)) \\ & \cap C([0, T]; H_{\text{per}}^1(D)) \cap C^1(0, T; L_{\text{per}}^2(D))\}. \end{aligned}$$

In order to derive existence and regularity results for (4.10), (4.11), we rewrite the model as an abstract parabolic equation in the form

$$\frac{\partial}{\partial t}(\delta^1, u^1) + \mathcal{A}(t)(\delta^1, u^1) = 0,$$

with the operators $\mathcal{A}(t) : H_{\text{per}}^2(D) \times H_{\text{per}}^1(D) \rightarrow L_{\text{per}}^2(D) \times H_{\text{per}}^{-1}(D)$ defined via

$$\mathcal{A}(t)(\delta^1, u^1) := \begin{pmatrix} -Lc_0\Delta\delta^1 + b^{-1}\rho^2c_0\delta^1 + b^{-1}\rho(\psi(\delta^0) - 2\mu^0\delta^0)\Delta u^1 \\ -b^{-1}(\psi(\delta^0) - \mu^0\delta^0)\Delta u^1 - b^{-1}\rho c_0\delta^1 \end{pmatrix}.$$

We start by verifying that $\mathcal{A}(t)$ is the generator of a parabolic evolution semigroup (cf. [1]) in the time interval $(0, T)$;

LEMMA 4.1. *There exists $\omega_0 \in \mathbb{C}$ such that, for each $t \in (0, T)$ and $\text{Re } \omega \geq \omega_0 > 0$, the operators*

$$(\omega I + \mathcal{A}(t)) : H_{\text{per}}^2(D) \times H_{\text{per}}^1(D) \rightarrow L_{\text{per}}^2(D) \times H_{\text{per}}^{-1}(D)$$

are continuous linear operators with bounded inverse. Moreover, the dependence of $\mathcal{A}(t)$ on t is Lipschitz in the time interval $(0, T)$.

Proof. The continuity of the operators $\omega I + \mathcal{A}(t)$ can be obtained from standard estimates on the defined spaces, and the Lipschitz-continuous dependence on t follows together with the Lipschitz-continuity of the coefficients. In order to verify the existence and boundedness of the inverse, we rewrite the equation $(\omega I + \mathcal{A}(t))(v, w) = (f, g)$ as

$$\mathcal{B}(t)(v, w) - \mathcal{C}(t)(v, w) = (f, g)$$

with the operators

$$\mathcal{B}(t)(v, w) := \begin{pmatrix} -Lc_0\Delta v + (\omega + b^{-1}\rho^2c_0)v + b^{-1}\rho(\psi(\delta^0) - 2\mu^0\delta^0)\Delta w \\ -b^{-1}(\psi(\delta^0) - \mu^0\delta^0)\Delta w + \omega w \end{pmatrix}$$

and

$$\mathcal{C}(t)(v, w) := \mathcal{B}(t)(v, w) - \mathcal{A}(t)(v, w) = (0, b^{-1}\rho c_0 v).$$

Since $\mathcal{B}(t)$ is a differential operator in triangular form, it is straight-forward to show that $\mathcal{B}(t)^{-1}$ exists and is continuous for $\text{Re } \omega > 0$. Moreover, from the compactness

of embedding operators we can deduce that $\mathcal{C}(t)$ is a compact operator, and hence, $\mathcal{B}(t)^{-1}\mathcal{C}(t)$ is compact. Thus, $(\omega I + \mathcal{A}(t))(v, w) = (f, g)$ is equivalent to

$$(I - \mathcal{B}(t)^{-1}\mathcal{C}(t))(v, w) = \mathcal{B}(t)^{-1}(v, w), \quad \text{in } H_{\text{per}}^2(D) \times H_{\text{per}}^1(D).$$

Since $I - \mathcal{B}(t)^{-1}\mathcal{C}(t)$ is a compact perturbation of the identity, it is continuously invertible if and only if it is injective (due to the Riesz-Schauder theory, cf. e.g. [33, Thm. 79.1]). We may conclude that $(\omega I + \mathcal{A}(t))$ has a continuous inverse if and only if it is injective.

Now assuming that $(\omega I + \mathcal{A}(t))(v, w) = 0$, then we can multiply the two equations with $(\bar{v}, -\Delta\bar{w})$, integrate over Ω , and add them to obtain (after applying Gauss' Theorem)

$$0 = \int_{\Omega} [Lc_0|\nabla v|^2 + (\omega + b^{-1}\rho^2c_0)|v|^2 + b^{-1}\rho(\psi(\delta^0) - 2\mu^0\delta^0)\Delta w\bar{v} \\ + b^{-1}(\psi(\delta^0) - \mu^0\delta^0)|\Delta w|^2 + \omega|\nabla w|^2 + b^{-1}\rho c_0v\Delta\bar{w}] dx.$$

By considering in particular the equation for the real part and applying the Cauchy-Schwarz inequality we deduce

$$0 \geq \int_{\Omega} [Lc_0|\nabla v|^2 + (\text{Re } \omega + b^{-1}\rho^2c_0 - b^{-1}\rho \frac{(c_0^2 + (\psi(\delta^0) - 2\mu^0\delta^0)^2)}{2(\psi(\delta^0) - \mu^0\delta^0)})|v|^2 \\ + (\text{Re } \omega|\nabla w|^2] dx.$$

If

$$\omega_0 \geq \max_{t \in [0, T]} b^{-1}\rho \frac{(c_0^2 + (\psi(\delta^0) - 2\mu^0\delta^0)^2)}{2(\psi(\delta^0) - \mu^0\delta^0)},$$

then we may conclude $v \equiv 0$ and $\nabla w \equiv 0$, which implies $w \equiv 0$ since $\int_D w dx = 0$. Thus, $\mathcal{A}(t)$ is injective, which completes the proof. \square

Since $\mathcal{A}(t)$ defines a parabolic evolution semigroup, we can now apply well-known results from linear parabolic theory (Theorem 1.2.1, p.43, and 1.2.2, p.44, in [1]) to conclude the following well-posedness result:

THEOREM 4.2. *Let $(\delta_0^1, u_0^1) \in L_{\text{per}}^2(D) \times H_{\text{per}}^1(D)$, let $(\delta^0, u^0) \in C^1([0, T])^2$ be the unique solution of (4.5), (4.6), and let (4.12) be satisfied. Then (4.8), (4.9) has a unique weak solution $(\delta^1, u^1) \in \mathcal{V}_{\text{per}}$, which depends continuously on the initial value.*

Linear stability of equilibria. In the following we study the linear stability of equilibria, i.e., the first-order expansion around a flat surface with vanishing adatom density. Since $\frac{du^0}{dt} = 0$ and $\delta^0 = 0$ at equilibrium, the system (4.8), (4.9) simplifies to

$$\frac{\partial \delta^1}{\partial t} - Lc_0\Delta\delta^1 + \rho \frac{\partial u^1}{\partial t} = 0 \tag{4.13}$$

$$b \frac{\partial u^1}{\partial t} - \Delta u^1 - \rho c_0\delta^1 = 0. \tag{4.14}$$

Multiplying (4.13) by $c_0\delta^1$ and (4.14) by $\frac{\partial u^1}{\partial t}$ and subsequent integration, we obtain the estimate

$$\frac{d}{dt} \left(\frac{c_0}{2} \int_D (\delta^1)^2 dx + \frac{1}{2} \int_D |\nabla u^1|^2 dx \right) \\ \leq -Lc_0^2 \int_D |\nabla \delta^1|^2 dx - b \int_D \left(\frac{\partial u^1}{\partial t} \right)^2 dx.$$

Inserting (4.14) at the right-hand side we deduce

$$\begin{aligned} b \int_D \left(\frac{\partial u^1}{\partial t} \right)^2 d\mathbf{x} &= b^{-1} \int_D (\Delta u^1 + \rho c_0 \delta^1)^2 d\mathbf{x} \\ &= b^{-1} \int_D [(\Delta u^1)^2 + 2\rho c_0 \Delta u^1 \delta^1 + \rho^2 c_0^2 (\delta^1)^2] d\mathbf{x} \\ &\geq b^{-1} \int_D \left[(1-\nu)(\Delta u^1)^2 + \left(1 - \frac{1}{\nu}\right) \rho^2 c_0^2 (\delta^1)^2 \right] d\mathbf{x} \end{aligned}$$

for arbitrary $\nu \in (0, 1)$. Moreover, due to Poincaré inequalities (note that δ^1 and u^1 have mean zero), there exists a constant $C > 0$ such that

$$\begin{aligned} \int_D |\nabla \delta^1|^2 d\mathbf{x} &\geq C \int_D (\delta^1)^2 d\mathbf{x} \\ \int_D (\Delta u^1)^2 d\mathbf{x} &\geq C \int_D |\nabla u^1|^2 d\mathbf{x}. \end{aligned}$$

Thus, we obtain the estimate

$$\begin{aligned} \frac{d}{dt} \left(\frac{c_0}{2} \int_D (\delta^1)^2 d\mathbf{x} + \frac{1}{2} \int_D |\nabla u^1|^2 d\mathbf{x} \right) &\leq -b^{-1}(1-\nu)C \int_D |\nabla u^1|^2 d\mathbf{x} \\ &\quad - \left(Lc_0C - b^{-1}\rho^2c_0^2\left(\frac{1}{\nu} - 1\right) \right) \int_D (\delta^1)^2 d\mathbf{x}. \end{aligned}$$

Thus, for $1-\nu$ sufficiently small there exists a constant c such that

$$\frac{d}{dt} E^1 \leq -cE^1$$

holds for the first-order expansion of the energy functional

$$E^1 := \frac{c_0}{2} \int_D (\delta^1)^2 d\mathbf{x} + \frac{1}{2} \int_D |\nabla u^1|^2 d\mathbf{x}.$$

As a direct consequence, we obtain the exponential decay of the energy E^1 and the exponential convergence $\delta^1 \rightarrow 0$ and $u^1 \rightarrow 0$. Hence, we may conclude linear stability of the equilibrium in the film case.

Local existence for the nonlinear problem. In the following we provide some partial existence results for (1.7), (1.8) for initial shapes sufficiently close to flat films, and initial adatom densities sufficiently close to constant densities. The main tool of this analysis is the implicit function theorem, to whose application the results of the previous section on the linearization (i.e., the first-order expansion) around special situations provide a basis. For the sake of simplicity we restrict our attention to the film case for dimension $d=1$ and assume without restriction of generality that $D=(0,1)$. Moreover, we assume for simplicity that $\mathbf{r}_{12}=0$.

The function space in which we look for a solution is given by

$$\begin{aligned} \mathcal{W}_{\text{per}} := \{ &(\delta, u) \mid \delta \in C([0, T]; H_{\text{per}}^1(D)) \cap C(0, T; H_{\text{per}}^2(D)) \\ &\cap C^1(0, T; H_{\text{per}}^1(D)), u \in C([0, T]; H_{\text{per}}^2(D)) \cap C(0, T; H_{\text{per}}^3(D)) \\ &\cap C^1(0, T; H_{\text{per}}^2(D)) \}, \end{aligned}$$

a choice which is motivated by the need to obtain $\delta \in C(D \times [0, T])$ and $Q = \sqrt{1 + |\nabla u|^2} \in C(D \times [0, T])$ via embedding. We can use this setting to obtain a local existence around flat initial surfaces and around constant initial adatom densities:

THEOREM 4.3. *Let $(\delta_0^0, u_0^0) \in \mathbb{R}_+^2$ satisfy $\psi(\delta_0^0) - \psi'(\delta_0^0)\delta_0^0 > 0$. Moreover, let $D = (0, 1)$, $r_3^0 \in C([0, t])$, $\mathbf{r}_{12} = 0$, and let $\epsilon > 0$ be arbitrary. Then there exists $T > 0$ and a constant $C_0 > 0$ such that for all initial values $(\delta_0, u_0) \in H_{\text{per}}^1(D) \times H_{\text{per}}^2(D)$ and right-hand sides $r_3 \in C^\epsilon([0, T]; H_{\text{per}}^1(D)) \cap C([0, T]; H_{\text{per}}^{1+\epsilon}(D))$ such that*

$$\|u_0 - u_0^0\|_{H^2} + \|\delta_0 - \delta_0^0\|_{H^1} + \|r_3 - r_3^0\| \leq C_0$$

there exists a locally unique solution $(u, \delta) \in \mathcal{W}_{\text{per}}$ of (2.9), (2.10) with initial value (u_0, δ_0) .

Proof. We give a sketch of the proof based on the Implicit Function Theorem in Banach spaces (cf. [19, Theorem 15.1]). First of all, one observes that (δ^0, u^0) is a spatially homogeneous solution of (2.9), (2.10) for the constant initial value (δ_0^0, u_0^0) . Moreover, with our choices of function spaces (and the embeddings $H_{\text{per}}^1(D) \hookrightarrow C(D)$ and $H_{\text{per}}^2(D) \hookrightarrow C^1(D)$ for $D = (0, 1)$) it is straight-forward to verify that the operators defining the left-hand side of (2.9), (2.10) are continuously Fréchet-differentiable in a neighbourhood of $(\delta^0, u^0; \delta_0^0, u^0, r_3^0)$. By analogous reasoning as in the proof of Theorem 4.2 (applying again Theorem 1.2.1, p.43, and 1.2.2, p.44, in [1], but with the function space setting of \mathcal{W}_{per}) one can show that the linearization of (2.9), (2.10) around $(\delta^0, u^0; \delta_0^0, u^0, r_3^0)$ is well-posed, i.e., the derivative of the equation operator with respect to (δ, u) has a continuous inverse. The implicit function theorem finally implies the existence of a locally unique solution. \square

Note that the result of Theorem 4.3 is still local in time, since the constant C_0 bounding the difference of initial values and deposition to the homogeneous case may depend on T . Since general flat surfaces are not stable, one has to expect blow-up of the solution to the first-order expansion and global existence cannot be obtained using the above techniques. The situation obviously differs close to equilibrium, since uniform estimates for the solutions of the linearized problem around equilibrium can be obtained.

THEOREM 4.4. *Let the assumptions of Theorem 4.3 be satisfied. Then there exists a constant $C_0 > 0$ such that for all $T > 0$, initial values $(\delta_0, u_0) \in H_{\text{per}}^1(D) \times H_{\text{per}}^2(D)$, and right-hand sides $r_3 \in C^\epsilon([0, T]; H_{\text{per}}^1(D)) \cap C([0, T]; H_{\text{per}}^{1+\epsilon}(D)) \cap L^2([0, T] \times D)$ satisfying*

$$\|u_0 - \frac{m}{|D|\rho}\|_{H^2} + \|\delta_0\|_{H^1} + \|r_3\| \leq C_0$$

there exists a unique solution $(u, \delta) \in \mathcal{W}_{\text{per}}$ of (2.9), (2.10) with initial value (u_0, δ_0) .

For the sake of brevity we just sketch the derivation of an a-priori estimate uniformly in time, the global existence of which can then be obtained together with Theorem 4.3. If u^1 and δ^1 denote the solution of (4.13) with right-hand side r_3 and (4.14), then for $\delta^0 = 0$, the functions $v := \frac{\partial \delta^1}{\partial x}$, $w := \frac{\partial u^1}{\partial x}$ solve

$$\begin{aligned} \frac{\partial v}{\partial t} - Lc_0 \frac{\partial^2 v}{\partial x^2} + \rho \frac{\partial w}{\partial t} &= \frac{\partial r_3}{\partial x} \\ b \frac{\partial w}{\partial t} - \frac{\partial^2 w}{\partial x^2} - \rho c_0 v &= 0. \end{aligned}$$

Multiplication of the equations with $c_0 v$ and $\frac{\partial w}{\partial t}$, addition and integration yields

$$\begin{aligned} & \frac{1}{2} \int_D (c_0 v(x, T)^2 + |\frac{\partial w}{\partial x}(x, T)|^2) dx - \frac{1}{2} \int_D (c_0 v(x, 0)^2 + |\frac{\partial w}{\partial x}(x, 0)|^2) dx \\ &= c_0 \int_0^T \int_D \frac{\partial r_3}{\partial x} v dx dt - \int_0^T \int_D (Lc_0^2 |\frac{\partial v}{\partial x}|^2 + b |\frac{\partial w}{\partial t}|^2) dx dt. \end{aligned}$$

By applying integration by parts and the Cauchy-Schwarz inequality to the first integral in the second line we deduce

$$\begin{aligned} & \frac{1}{2} \int_D (c_0 v(x, T)^2 + |\frac{\partial w}{\partial x}(x, T)|^2) dx + \int_0^T \int_D (\frac{Lc_0^2}{2} |\frac{\partial v}{\partial x}|^2 + b |\frac{\partial w}{\partial t}|^2) dx dt \\ & \leq \frac{1}{2} \int_D (c_0 v(x, 0)^2 + |\frac{\partial w}{\partial x}(x, 0)|^2) dx + \frac{1}{2L} \int_0^T \int_D (r_3)^2 dx dt, \end{aligned}$$

which provides a uniform estimate in T .

We finally mention that in the case $r_3 \equiv 0$, the above estimate for v and w can be used together with a Poincaré-inequality to obtain exponential decay of v and w in time. In order to obtain a result on the decay of the solutions (δ, u) of (2.9), (2.10), we shall investigate the decay of the energy below.

Long-time behaviour of the nonlinear model. We now turn our attention to the long-time asymptotics of the nonlinear model (2.9), (2.10), again restricting our attention to the case $D = (0, 1) \subset \mathbb{R}^1$ for simplicity. We consider solutions such that $\frac{\partial u}{\partial x}$ is globally bounded in $L^\infty(D \times \mathbb{R}_+)$ and hence, there exists a constant c_Q such that

$$1 \leq Q(x, t) = \sqrt{1 + \left(\frac{\partial u}{\partial x}\right)^2} \leq c_Q, \quad \forall x \in D, t \in \mathbb{R}_+. \quad (4.15)$$

Note that due to the continuous embedding $H^2(D) \hookrightarrow C^1(D)$ in the case $D \subset \mathbb{R}^1$, the global existence of such solutions with uniform bound is guaranteed by Theorem 4.4.

The basic quantity, whose decay we shall study in the following, is the energy difference

$$e(t) := E(\delta(t), u(t)) - E(\hat{\delta}, \hat{u}) = \int_D [\psi(\delta(x, t))Q(x, t) - 1] dx.$$

From the energy dissipation relation we deduce as above

$$\frac{de}{dt} = - \int_D \left[\frac{L}{Q^3} \left(\frac{\partial \mu}{\partial x}\right)^2 + \frac{b}{Q} \left(\frac{\partial u}{\partial t}\right)^2 \right] dx. \quad (4.16)$$

In order to obtain exponential decay of e , we need to estimate the right-hand side from above by $-c_0 e$ for some constant $c_0 \in \mathbb{R}_+$, which is again mainly based on Poincaré inequalities.

THEOREM 4.5. *Let $\mathbf{r} \equiv 0$ and let $(\delta, u) \in C(\mathbb{R}_+; H^1(D)) \cap C(\mathbb{R}_+; H^2(D))$ be a nonnegative solution of (2.9), (2.10) on $D = (0, 1)$ satisfying (4.15) and*

$$\psi(\delta(x, t)) - \delta(x, t)\mu(x, t) \geq a, \quad \forall (x, t) \in D \times \mathbb{R}_+ \quad (4.17)$$

for some $a > 0$. Then there exist constants $c_0 > 0$ and $c_1 > 0$ such that

$$E(\delta(t), u(t)) \leq E(\hat{\delta}, \hat{u}) + E(\delta(0), u(0))e^{-c_0 t} \quad (4.18)$$

and

$$\int_D \delta^2 dx + \int_D \left(\frac{\partial u}{\partial x} \right)^2 dx \leq c_1 e^{-c_0 t}. \quad (4.19)$$

Proof. We start by estimating the right-hand side of (4.16). Inserting (2.10) we obtain

$$\begin{aligned} \int_D \frac{b}{Q} \left(\frac{\partial u}{\partial t} \right)^2 dx &= \int_D \frac{1}{bQ^5} \left[(\psi(\delta) - \delta\mu) \frac{\partial^2 u}{\partial x^2} - \rho\mu Q^3 \right]^2 dx \\ &\geq \int_D \frac{\epsilon}{bQ^5} \left[(\psi(\delta) - \delta\mu) \frac{\partial^2 u}{\partial x^2} - \rho\mu Q^3 \right]^2 dx \\ &= \int_D \frac{\epsilon}{bQ^5} \left[(\psi(\delta) - \delta\mu)^2 \left(\frac{\partial^2 u}{\partial x^2} \right)^2 + \rho^2 \mu^2 Q^6 \right] dx \\ &\quad - 2\frac{\epsilon}{b} \int_D (\psi(\delta) - \delta\mu) \frac{\partial}{\partial x} \left(\arctan \frac{\partial u}{\partial x} \right) \rho\mu dx \end{aligned}$$

for any $\epsilon \in (0, 1)$. Since u is periodic, $\frac{\partial u}{\partial x}$ has mean zero, and we may therefore apply the Poincaré inequality to obtain an estimate of the form

$$\tilde{c} \int_D \left(\frac{\partial u}{\partial x} \right)^2 dx \leq \int_D \left(\frac{\partial^2 u}{\partial x^2} \right)^2 dx$$

for some constant $\tilde{c} > 0$. From the nonnegativity of δ , (4.17) and the convexity of ψ we deduce

$$|\psi(\delta) - 2\delta\mu| \leq |\psi(\delta) - \delta\mu| \leq \psi(0) = 1$$

and hence, using integration by parts (and periodicity of u and δ to cancel the boundary terms)

$$\begin{aligned} &-2\frac{\epsilon}{b} \int_D (\psi(\delta) - \delta\mu) \frac{\partial}{\partial x} \left(\arctan \frac{\partial u}{\partial x} \right) \rho\mu dx \\ &= 2\frac{\epsilon\rho}{b} \int_D (\psi(\delta) - 2\delta\mu) \frac{\partial\mu}{\partial x} \arctan \frac{\partial u}{\partial x} dx \geq -2\frac{\epsilon\rho}{b} \int_D \left| \frac{\partial\mu}{\partial x} \right| \left| \frac{\partial u}{\partial x} \right| dx \\ &\geq -\frac{\epsilon a^2}{2bc_Q^5} \tilde{c} \int_D \left(\frac{\partial u}{\partial x} \right)^2 dx - \frac{2\epsilon\rho^2 c_Q^5}{a^2 b \tilde{c}} \int_D \left(\frac{\partial\mu}{\partial x} \right)^2 dx \end{aligned}$$

Using (4.15), (4.17), and the Poincaré inequality we further deduce

$$\int_D \frac{b}{Q} \left(\frac{\partial u}{\partial t} \right)^2 dx \geq \frac{\epsilon}{b} \int_D \left[\frac{a^2 \tilde{c}}{2c_Q^5} \left(\frac{\partial u}{\partial x} \right)^2 + c_Q \rho^2 \mu^2 - \frac{2\rho^2 c_Q^5}{a^2 \tilde{c}} \left(\frac{\partial\mu}{\partial x} \right)^2 \right] dx,$$

and hence,

$$\frac{de}{dt} \leq -\frac{\epsilon}{b} \int_D \left[\frac{a^2 \tilde{c}}{2c_Q^5} \left(\frac{\partial u}{\partial x} \right)^2 + c_Q \rho^2 \mu^2 + \left(\frac{bL}{\epsilon C_Q^3} - \frac{2\rho^2 c_Q^5}{a^2 \tilde{c}} \right) \left(\frac{\partial\mu}{\partial x} \right)^2 \right] dx.$$

Choosing $0 < \epsilon < \frac{a^2 b L \tilde{c}}{2 \rho^2 c_Q^2}$ we obtain an estimate of the form

$$\frac{de}{dt} \leq -\hat{c} \int_D \left[\left(\frac{\partial u}{\partial x} \right)^2 + \mu^2 \right] dx. \quad (4.20)$$

Using the properties of the maps $\frac{\partial u}{\partial x} \mapsto Q$ and $\delta \mapsto \psi(\delta)$ (convexity, values and derivatives at $\delta=0$ and $\frac{\partial u}{\partial x}=0$), we deduce

$$\begin{aligned} e &= \int_D (\psi(\delta) - 1) Q \, dx + \int_D (Q - 1) \, dx \\ &\geq \int_D (\psi(\delta) - 1) \, dx + \int_D (Q - 1) \, dx \\ &\geq C \left[\int_D \delta^2 \, dx + \int_D \left(\frac{\partial u}{\partial x} \right)^2 \, dx \right] \end{aligned}$$

for some constants $C, \tilde{C} > 0$. Together with (4.20) we can now conclude

$$\frac{de}{dt}(t) \leq -c_0 e(t)$$

for almost any t and the Gronwall Lemma implies (4.18). Moreover, the above lower bound on e implies (4.19). \square

We finally mention that in the case of the assumptions on the solution made in Theorem 4.5, namely (4.15) and (4.17), are satisfied at least if the initial value is sufficiently close to equilibrium in the sense of Theorem 4.4. For a constant C_0 sufficiently small, the uniform bounds on the linearization can be used to obtain (4.15) and a uniform bound of the form $0 \leq \delta \leq C_0 C_1$ for all $t > 0$. Consequently, we can estimate

$$\psi(\delta) - \delta \mu \geq 1 - C_0^2 C_2$$

for some constant C_2 , and for C_0 sufficiently small this implies (4.17).

4.2. Crystals close to radial symmetry. We now consider the dynamics for a crystal structure in \mathbb{R}^2 close to radial symmetry, without restriction of generality centered at the origin. The angular variable will be denoted by θ . We consider a deposition flux being homogeneous in the radial direction, i.e., $\mathbf{r} = r_0(t) \frac{\mathbf{x}}{|\mathbf{x}|}$. We assume that the initial value satisfies

$$\delta_0(\mathbf{x}) = \delta_0^0 + \epsilon \delta_0^1(\mathbf{x}) + \mathcal{O}(\epsilon^2) \quad (4.21)$$

$$\mathbf{x}_0(\theta) = R_0^0(\cos \theta, \sin \theta) + \epsilon \mathbf{x}_0^1(\theta) + \mathcal{O}(\epsilon^2) \quad (4.22)$$

and look for solutions in an expansion of the form

$$\delta(\theta, t) = \delta^0(t) + \epsilon \delta^1(\theta, t) + \mathcal{O}(\epsilon^2) \quad (4.23)$$

$$\mathbf{x}(\theta, t) = R^0(t)(\cos \theta, \sin \theta) + \epsilon \mathbf{x}^1(\theta, t) + \mathcal{O}(\epsilon^2). \quad (4.24)$$

We look in particular for an expansion such that the arclength is unchanged to first order, i.e.,

$$\left| \frac{\partial \mathbf{x}}{\partial \theta} \right| = R^0(t) + \mathcal{O}(\epsilon^2),$$

which leads to the condition

$$\frac{\partial x_1^1}{\partial \theta} \sin \theta - \frac{\partial x_2^1}{\partial \theta} \cos \theta = 0 \quad (4.25)$$

for the first-order expansion of the parametrization $\mathbf{x}^1 = (x_1^1, x_2^1)$.

Lowest order expansion. In order to obtain the lowest order expansion of (1.7), (1.8) in the above parametrization we notice that the curvature is given by

$$\kappa = -\frac{1}{R^0(t)} + \frac{\epsilon}{R^0(t)^2} \left(\frac{\partial^2 x_1^1}{\partial \theta^2} \cos \theta + \frac{\partial x_2^1}{\partial \theta^2} \sin \theta \right) + \mathcal{O}(\epsilon^2),$$

and the normal velocity can be expanded as

$$V = \frac{dR^0}{dt} + \epsilon \left(\frac{\partial x_1^1}{\partial t} \cos \theta + \frac{\partial x_2^1}{\partial t} \sin \theta \right) + \mathcal{O}(\epsilon^2).$$

The derivatives with respect to the shape variable S turn to derivatives with respect to the angular variable θ , which vanish at lowest order. Thus, the lowest order expansion is determined by

$$\frac{d\delta^0}{dt} + \left(\rho + \frac{\delta^0}{R^0} \right) \frac{dR^0}{dt} = r_0 \quad (4.26)$$

$$b \frac{dR^0}{dt} + \frac{\psi(\delta^0)}{R^0} - \left(\rho + \frac{\delta^0}{R^0} \right) \psi'(\delta^0) = 0. \quad (4.27)$$

We shall use the notation $\mu^0 = \psi'(\delta^0)$ for the chemical potential corresponding to δ^0 . The conservation of the total mass

$$m(t) = 2R^0 \pi \delta^0 + (R^0)^2 \pi \rho$$

is described by (4.26), which is equivalent to

$$\frac{dm}{dt} = 2R^0 \pi r_0,$$

i.e., the change of mass is proportional to the mass flow over the surface. In a similar way, we have dissipation of the lowest order expansion of the surface energy

$$E^0(t) = 2R^0 \pi \psi(\delta^0),$$

which we obtain as

$$\frac{dE^0}{dt} = -2R^0 \pi b \left(\frac{dR^0}{dt} \right)^2 + 2R^0 \pi r_0 \mu^0.$$

In particular, we obtain a decrease of the surface energy at constant mass in the absence of deposition.

THEOREM 4.6. *For all initial values $(\delta_0^0, R_0^0) \in \mathbb{R}_+^2$ with $R_0 > 0$ and each $r_0 \in C([0, T])$, there exists a unique solution $(\delta^0, R^0) \in C^1([0, T])^2$ of (4.26), (4.27) with $R^0(t) > 0$ for all $t \in [0, T]$.*

Proof. We insert (4.27) into (4.26), and equivalently rewrite the system as

$$\begin{aligned}\frac{d\delta^0}{dt} &= b^{-1} \left(\rho + \frac{\delta^0}{R^0} \right) \left(\frac{\psi(\delta^0)}{R^0} - \left(\rho + \frac{\delta^0}{R^0} \right) \psi'(\delta^0) \right) + r_0 \\ \frac{dR^0}{dt} &= b^{-1} \frac{\psi(\delta^0)}{R^0} - b^{-1} \left(\rho + \frac{\delta^0}{R^0} \right) \psi'(\delta^0).\end{aligned}$$

Now let $f := \frac{1}{R^0}$, then we can seek (δ^0, f) equivalently as a solution of

$$\begin{aligned}\frac{d\delta^0}{dt} &= b^{-1} (\rho + f\delta^0) (f\psi(\delta^0) - (\rho + f\delta^0)\psi'(\delta^0)) + r_0 \\ \frac{df}{dt} &= -b^{-1} f^3 \psi(\delta^0) + b^{-1} f^2 (\rho + f\delta^0) \psi'(\delta^0).\end{aligned}$$

Since the right-hand side is continuous and a C^1 -function of (δ^0, f) we may conclude existence and uniqueness of a solution $(\delta^0, f) \in C^1([0, T])^2$ from the Picard-Lindelöf Theorem for ordinary differential equations. It suffices to show that $f > 0$ to conclude the assertion. On the other hand the identity

$$\frac{dR^0}{dt} = b^{-1} f\psi(\delta^0) - b^{-1} (\rho + f\delta^0) \psi'(\delta^0)$$

implies the boundedness of $R_0 = \frac{1}{f}$ and $\frac{dR^0}{dt}$. Hence, there exists a solution $R_0 \in C^1([0, T])$ such that $R_0(t) > 0$ for all $t \in [0, T]$. \square

In the film case, we have seen that the lowest order expansion of the adatom density decays to zero exponentially. In the crystal case we cannot expect such behaviour, since the adatom density does not vanish at equilibrium. One would rather expect that the adatom density will be bounded away from zero for all times if

$$\delta_0^0 > 0 \quad \text{and} \quad r_0(t) > 0, \quad \forall t \geq 0. \quad (4.28)$$

This can be seen as follows: since $\psi(\delta^0) \geq \psi(0) = 1$ and $R^0(t)$ is bounded, there exists a constant $C > 0$ (depending on T , δ_0^0 , and R^0) such that

$$\psi(\delta^0) - R^0 \rho \psi'(\delta^0) - \delta^0 \psi'(\delta^0) \geq 1 - C \rho \psi'(\delta^0) - \delta^0 \psi'(\delta^0),$$

and because $\psi'(\delta^0) \rightarrow 0$ as $\delta^0 \rightarrow 0$, there exists a constant $\alpha > 0$ (depending again on T , δ_0^0 , and R^0) such that

$$\psi(\delta^0) - R^0 \rho \psi'(\delta^0) - \delta^0 \psi'(\delta^0) \geq 0$$

for $\delta^0 \leq \alpha$. With the ordinary differential equation for δ^0 we conclude that

$$\frac{d\delta^0}{dt} = b^{-1} \left(\rho + \frac{\delta^0}{R^0} \right) \left(\frac{\psi(\delta^0)}{R^0} - \left(\rho + \frac{\delta^0}{R^0} \right) \psi'(\delta^0) \right) + r_0 \geq r_0 \geq 0$$

if $\delta^0(t) \leq \alpha$. Hence, under the assumption (4.28) we may conclude the lower bound $\delta^0(t) \geq \min\{\delta_0^0, \alpha\} > 0$ for all $t \in [0, T]$.

We can use similar reasoning to show that the effective diffusion coefficient $\psi(\delta^0) - \psi'(\delta^0)\delta^0$, which we will meet again in the first-order expansion, is bounded away from zero if $\psi(\delta_0^0) - \psi'(\delta_0^0)\delta_0^0 > 0$ and $r_0 \equiv 0$.

First order expansion. In order to simplify the analysis of the first order expansion problem for (1.7), (1.8), we introduce the variable

$$w^1 := x_1^1 \cos \theta + x_2^1 \sin \theta. \quad (4.29)$$

We have

$$\frac{\partial w^1}{\partial t} = \frac{\partial x_1^1}{\partial t} \cos \theta + \frac{\partial x_2^1}{\partial t} \sin \theta$$

and thus, $\frac{\partial w^1}{\partial t}$ equals the first-order expansion of the normal velocity. Moreover,

$$\frac{\partial^2 w^1}{\partial \theta^2} = \frac{\partial^2 x_1^1}{\partial \theta^2} \cos \theta + \frac{\partial^2 x_2^1}{\partial \theta^2} \sin \theta - x_1^1 \cos \theta - x_2^1 \sin \theta,$$

from which we conclude that the first-order expansion of the mean curvature is given by

$$\kappa = -\frac{1}{R^0} + \frac{\epsilon}{(R^0)^2} \left(\frac{\partial^2 w^1}{\partial \theta^2} + w^1 \right) + \mathcal{O}(\epsilon^2).$$

We can ignore the first order expansion of the tangential velocity, since the surface gradient of δ^0 vanishes and thus $\mathbf{v} \cdot \nabla \delta = \mathcal{O}(\epsilon^2)$.

Using these relations for normal velocity and mean curvature, we derive the following equations for the first-order terms

$$\begin{aligned} \frac{\partial \delta^1}{\partial t} - \frac{Lc_0}{(R^0)^2} \frac{\partial^2 \delta^1}{\partial \theta^2} + \left(\rho + \frac{\delta^0}{R^0} \right) \frac{\partial w^1}{\partial t} + \frac{\delta^1}{R^0} \frac{dR^0}{dt} \\ - \frac{\delta^0}{(R^0)^2} \frac{dR^0}{dt} \left(\frac{\partial^2 w^1}{\partial \theta^2} + w^1 \right) = 0, \end{aligned} \quad (4.30)$$

$$\frac{\partial w^1}{\partial t} - \frac{\psi^0 - \delta^0 \mu^0}{(R^0)^2} \left(\frac{\partial^2 w^1}{\partial \theta^2} + w^1 \right) - c_0 \left(\rho + \frac{\delta^0}{R^0} \right) \delta^1 = 0. \quad (4.31)$$

The analysis of this first-order expansion (4.30), (4.31) can be carried in the space

$$\begin{aligned} \mathcal{V}_{\text{per}} := \{ (\delta^1, w^1) \mid \delta^1 \in C(0, T; H_{\text{per}}^1([0, 2\pi])) \cap C([0, T]; L_{\text{per}}^2([0, 2\pi])) \\ \cap C^1(0, T; H_{\text{per}}^{-1}([0, 2\pi])), \quad w^1 \in C(0, T; H_{\text{per}}^2([0, 2\pi])) \\ \cap C([0, T]; H_{\text{per}}^1([0, 2\pi])) \cap C^1(0, T; L_{\text{per}}^2([0, 2\pi])) \}. \end{aligned}$$

Since the proof of existence and uniqueness can be carried out in an analogous way to the analysis of the first order expansion in the film case, we only state the corresponding result:

THEOREM 4.7. *Let $(\delta_0^1, w_0^1) \in L_{\text{per}}^2([0, 2\pi]) \times H_{\text{per}}^1([0, 2\pi])$, and let $(\delta^0, R^0) \in C^1([0, T])^2$ be the unique solution of (4.26), (4.27) with positive initial values and $r_0 \geq 0$. Moreover, let $\psi(\delta^0(t)) - \delta^0(t)\mu^0(t) \geq a$, be satisfied for some $a > 0$ and all $t \in [0, T]$. Then (4.30), (4.31) has a unique weak solution $(\delta^1, w^1) \in \mathcal{V}_{\text{per}}$, which depends continuously on the initial value.*

Theorem 4.7 guarantees the existence and uniqueness of the adatom density and of the transformed variable w^1 , it remains to reconstruct the first-order expansion \mathbf{x}^1 of the surface parametrization from w^1 . From (4.25) and the definition of w^1 we have

$$\frac{\partial}{\partial \theta} (x_1^1 \sin \theta - x_2^1 \cos \theta) = x_1^1 \cos \theta + x_2^1 \sin \theta + \frac{\partial x_1^1}{\partial \theta} \sin \theta - \frac{\partial x_2^1}{\partial \cos} \theta = w^1.$$

We can integrate with respect to θ to obtain

$$x_1^1 \sin \theta - x_2^1 \cos \theta = \int_0^\theta w^1 d\zeta.$$

We can use this relation together with the definition of w^1 to compute the first-order expansion of the parametrization as

$$\mathbf{x}^1(\theta, t) = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix} \begin{pmatrix} w^1(\theta, t) \\ \int_0^\theta w^1(\zeta, t) d\zeta \end{pmatrix}.$$

Linear stability of radially symmetric equilibria. We can now investigate the linear stability of a radially symmetric equilibrium, the linearized model which is given by

$$\frac{\partial \delta^1}{\partial t} - \frac{Lc_0}{(R^0)^2} \frac{\partial^2 \delta^1}{\partial \theta^2} + \left(\rho + \frac{\delta^0}{R^0}\right) \frac{\partial w^1}{\partial t} = 0, \quad (4.32)$$

$$\frac{\partial w^1}{\partial t} - \frac{\psi^0 - \delta^0 \mu^0}{(R^0)^2} \left(\frac{\partial^2 w^1}{\partial \theta^2} + w^1 \right) - c_0 \left(\rho + \frac{\delta^0}{R^0} \right) \delta^1 = 0. \quad (4.33)$$

By completely analogous reasoning to the film case we can derive an estimate of the form

$$\frac{dE^1}{dt}(t) \leq -cE^1(t), \quad \forall t \in (0, T),$$

where E^1 is the first-order expansion of the energy, given by

$$E^1(t) := \int_0^{2\pi} \left[c_0 (\delta^1)^2 + \left(\frac{\partial w^1}{\partial \theta} \right)^2 - (w^1)^2 \right] d\theta.$$

Thus, we again obtain exponential decay of E^1 . Since the smallest eigenvalue of the operator $w \mapsto -\frac{\partial^2 w}{\partial \theta^2}$ in $L^2_{\text{per}}([0, 2\pi])$ is equal to 1, we obtain that

$$\int_0^{2\pi} \left[\left(\frac{\partial w^1}{\partial \theta} \right)^2 - (w^1)^2 \right] d\theta \geq 0.$$

Equality would imply that w^1 is a linear combination of the functions $\sin \theta$ and $\cos \theta$, and consequently that x_1^1 and x_2^1 are constant, which is impossible for the first-order expansion unless $\mathbf{x}^1 \equiv 0$. Hence, the decay of E^1 implies that δ^1 and w^1 converge to zero, and thus, linear stability of the radial equilibrium.

Nonlinear dynamics of star-shaped crystals. In order to gain some insight into the nonlinear dynamics in the crystal case, we consider a star-shaped crystal in the plane, i.e.,

$$\mathbf{x}(t) = e^{u(\theta, t)} (\cos \theta, \sin \theta), \quad \theta \in [0, 2\pi],$$

with a periodic function u . Moreover, we assume that the deposition can be written as

$$\mathbf{r} = r_{rad}(\cos \theta, \sin \theta),$$

with a nonnegative, periodic scalar function r_{rad} . The normal velocity V and the mean curvature κ can be expressed as

$$V = \frac{e^u}{Q} \frac{\partial u}{\partial t}, \quad \kappa = \frac{1}{e^u Q^3} \left(\frac{\partial^2 u}{\partial \theta^2} - Q^2 \right) \quad (4.34)$$

where

$$Q := \sqrt{1 + \left(\frac{\partial u}{\partial \theta} \right)^2}. \quad (4.35)$$

The model (1.7), (1.8) can be rewritten in terms of u and an adatom density δ being a function θ as

$$\begin{aligned} \frac{\partial \delta}{\partial t} Q - \frac{1}{Q} \frac{\partial u}{\partial t} \frac{\partial u}{\partial \theta} \frac{\partial \delta}{\partial \theta} - e^{-u} \frac{\partial}{\partial \theta} \left(\frac{L e^{-u}}{Q} \frac{\partial \mu}{\partial \theta} \right) \\ + (\rho e^u - \frac{\delta}{Q^3} (\frac{\partial^2 u}{\partial \theta^2} - Q^2)) \frac{\partial u}{\partial t} = r_{rad} \end{aligned} \quad (4.36)$$

$$b e^u \frac{\partial u}{\partial t} - (\psi - \delta \mu) e^{-u} \left(\frac{1}{Q^2} \frac{\partial^2 u}{\partial \theta^2} - 1 \right) - \rho \mu Q = 0, \quad (4.37)$$

in $(0, 2\pi) \times (0, T)$. The associated surface energy is given by

$$\tilde{E}(u, \delta) := E(\Gamma, \delta) = \int_0^{2\pi} \psi(\delta) e^u Q \, d\theta. \quad (4.38)$$

At constant mass

$$\tilde{m}(u, \delta) = \int_0^{2\pi} \delta e^u Q \, d\theta,$$

there exists a global energy minimizer of radial shape and constant adatom density due to Theorem 3.5, which we shall denote by the constant $(\hat{u}, \hat{\delta})$.

The lowest order expansion around a radial shape (u^0 constant) and constant adatom density δ^0 is given by (4.26), (4.27) with $u^0 = \log R^0$. Besides the exponential terms e^u , the model (4.36), (4.37) has a similar structure to the film case (2.9), (2.10). Therefore it is not surprising that the proof of local existence close to spatially homogeneous adatom densities and radial shapes (i.e. flat graphs u) can be carried out in an analogous way as the proof of Theorem 4.3. The additional exponential terms do not appear in the linearization and their derivatives can be handled in a straight-forward way due to the strong regularity we use. Around equilibrium $(\hat{u}, \delta u)$ and vanishing deposition $r_{rad} = 0$, global bounds can be derived as in the film case in Theorem 4.4 and hence, we can derive the following existence result:

THEOREM 4.8. *Let $(\delta_0^0, u_0^0) \in \mathbb{R}_+^2$ and let (δ^0, e^{u^0}) be a solution of (4.26), (4.27) satisfying $\psi(\delta^0(t)) - \delta^0(t) \mu^0(t) \geq a$, for some $a > 0$ and all $t \in [0, T]$. Moreover, let $D = (0, 2\pi)$, $r_{rad}^0 \in C([0, t])$, and let $\epsilon > 0$ be arbitrary. Then there exists $T > 0$ and a constant $C_0 > 0$ such that for all initial values $(\delta_0, u_0) \in H_{per}^1(D) \times H_{per}^2(D)$ and right-hand sides*

$$r_{rad} \in C^\epsilon([0, T]; H_{per}^1(D)) \cap C([0, T]; H_{per}^{1+\epsilon}(D))$$

such that

$$\|u_0 - u_0^0\|_{H^2} + \|\delta_0 - \delta_0^0\|_{H^1} + \|r_{rad} - r_{rad}^0\| \leq C_0$$

there exists a locally unique solution $(u, \delta) \in \mathcal{W}_{per}$ of (4.36), (4.37) with initial value (u_0, δ_0) .

If, in addition, $(u_0^0, \delta_0^0) = (\hat{u}, \hat{\delta})$ and $r_{rad}^0 = 0$, then the existence is global in time with uniform bounds in T .

Opposed to existence and uniqueness, the characterization of long time behaviour is different to the film case, since the structure of equilibria differs due to $\hat{\delta} \neq 0$. As a consequence we cannot derive exponential decay from the energy alone, but instead we have to consider the Lagrangian

$$L(u, \delta; \lambda) = \tilde{E}(u, \delta) + \lambda(m(u, \delta) - m_0),$$

with scalar parameter λ . Note that at equilibrium we have

$$0 = \frac{\partial L}{\partial \delta}(\hat{u}, \hat{\delta}; \hat{\lambda}) \eta = \int_0^{2\pi} (\hat{\mu} + \hat{\lambda}) \eta e^{\hat{u}} Q \, d\theta,$$

at least for each constant η and hence, the equilibrium Lagrange parameter is given by $\hat{\lambda} = -\hat{\mu} = -\psi'(\hat{\delta})$. Since the mass is conserved during the evolution, we obtain

$$\frac{dt}{dt} L(u(t), \delta(t); \hat{\lambda}) = \frac{dt}{dt} \tilde{E}(u(t), \delta(t)).$$

Thus, we can alternatively use the Lagrangian L for the decay estimate, and as we shall prove in the following, L can be estimated from below close to equilibrium:

LEMMA 4.2. *Let $(\hat{u}, \hat{\delta})$ be the minimizer of \tilde{E} at fixed mass $\tilde{m} = m_0$, being constant according to Theorem 3.5. Then there exists a constant $C_1 > 0$ such that*

$$L(u, \delta, \hat{\lambda}) - L(\hat{u}, \hat{\delta}, \hat{\lambda}) \geq C_1 \int_0^{2\pi} \left((\delta - \hat{\delta})^2 + (u - \hat{u})^2 + \left(\frac{\partial u}{\partial \theta} - \frac{\partial \hat{u}}{\partial \theta} \right)^2 \right) d\theta$$

for all $(u, \delta) \in H_{per}^2(D) \times H_{per}^1(D)$ with $\|u - \hat{u}\|_{H^2} + \|\delta - \hat{\delta}\|_{H^2}$ sufficiently small.

Proof. We start by computing second derivatives of L at equilibrium

$$\begin{aligned} \frac{\partial^2}{\partial u^2} L(\hat{u}, \hat{\delta}; \hat{\lambda})(\varphi, \varphi) &= \int_0^{2\pi} (\psi(\hat{\delta}) + \hat{\lambda} \hat{\delta}) e^{\hat{u}} \left(\varphi^2 + \left(\frac{\partial \varphi}{\partial \theta} \right)^2 \right) d\theta \\ \frac{\partial^2}{\partial u \partial \delta} L(\hat{u}, \hat{\delta}; \hat{\lambda})(\varphi, \eta) &= \int_0^{2\pi} (\hat{\mu} + \hat{\lambda}) \varphi \eta e^{\hat{u}} d\theta \\ \frac{\partial^2}{\partial \delta^2} L(\hat{u}, \hat{\delta}; \hat{\lambda})(\eta, \eta) &= \int_0^{2\pi} \psi''(\hat{\delta}) \eta^2 e^{\hat{u}} d\theta. \end{aligned}$$

Since $\hat{\lambda} = -\hat{\mu}$, the mixed derivative $\frac{\partial^2}{\partial u \partial \delta} L(\hat{u}, \hat{\delta}; \hat{\lambda})$ vanishes and hence, if $\psi(\hat{\delta}) + \hat{\lambda} \hat{\delta} = \psi(\hat{\delta}) - \hat{\mu} \hat{\delta}$ is positive, we can find a constant C_0 such that

$$L''(\hat{u}, \hat{\delta}; \hat{\lambda})(\varphi, \eta)^2 \geq C_0 \int_0^{2\pi} \left(\varphi^2 + \left(\frac{\partial \varphi}{\partial \theta} \right)^2 + \eta^2 \right) d\theta.$$

Thus, L is locally strictly convex around $(\hat{u}, \hat{\delta})$, which implies the assertion. \square

Now we are in position to derive an exponential decay result for the adatom density and the parametrization u locally around equilibrium:

THEOREM 4.9. *Let $\mathbf{r} \equiv 0$ and let $(\delta, u) \in C(\mathbb{R}_+; H^1(D)) \cap C(\mathbb{R}_+; H^2(D))$ be a solution of (2.9), (2.10) on $D = (0, 2\pi)$ satisfying $\delta \geq 0$ and*

$$\psi(\delta(x, t)) - \delta(x, t)\mu(x, t) \geq a, \quad \forall (x, t) \in D \times \mathbb{R}_+ \quad (4.39)$$

for some $a > 0$. Then there exist constants $c_0 > 0$ and $c_1 > 0$ such that

$$L(u(t), \delta(t), \hat{\lambda}) \leq L(\hat{u}, \hat{\delta}, \hat{\lambda}) + L(u(0), \delta(0), \hat{\lambda})e^{-c_0 t} \quad (4.40)$$

and

$$\int_0^{2\pi} \left((\delta - \hat{\delta})^2 + (u - \hat{u})^2 + \left(\frac{\partial u}{\partial \theta} - \frac{\partial \hat{u}}{\partial \theta} \right)^2 \right) d\theta \leq c_1 e^{-c_0 t}. \quad (4.41)$$

Proof. A similar calculation to the proof of Theorem 4.5 yields

$$\frac{dt}{dt} L(u(t), \delta(t), \hat{\lambda}) = -b \int_0^{2\pi} \frac{e^{3u}}{Q} \left(\frac{\partial u}{\partial t} \right)^2 d\theta - \int_0^{2\pi} \frac{Le^{-u}}{Q} \left(\frac{\partial \mu}{\partial \theta} \right)^2 d\theta.$$

By inserting (4.37), using the uniform estimates for u and Q , and analogous reasoning as in the proof of Theorem 4.5, we derive an estimate of the form

$$\frac{dt}{dt} L(u(t), \delta(t), \hat{\lambda}) \leq -C_2 \int_0^{2\pi} \left[\left(\frac{\partial \mu}{\partial \theta} \right)^2 + \left(\frac{\partial^2 u}{\partial \theta^2} - Q^2 \right)^2 \right] d\theta.$$

The second term can be estimated via

$$\begin{aligned} \int_0^{2\pi} \left(\frac{\partial^2 u}{\partial \theta^2} - Q^2 \right)^2 d\theta &= \int_0^{2\pi} \left[\left(\frac{\partial^2 u}{\partial \theta^2} \right)^2 - 2Q^2 \frac{\partial^2 u}{\partial \theta^2} + Q^4 \right] d\theta \\ &\geq \int_0^{2\pi} \left[-\frac{\partial}{\partial \theta} \left(\frac{\partial u}{\partial \theta} + \frac{1}{3} \left(\frac{\partial u}{\partial \theta} \right)^3 \right) + Q^2 \right] d\theta \\ &= \int_0^{2\pi} Q d\theta \geq C_3 \int_0^{2\pi} (\psi(\delta) + \hat{\lambda}\delta) e^u Q d\theta, \end{aligned}$$

where we have used the fact that $Q \geq 1$ and the uniform bounds for u and δ . Hence,

$$\frac{dt}{dt} L(u(t), \delta(t), \hat{\lambda}) \leq -c_0 L(u(t), \delta(t), \hat{\lambda}),$$

which implies the exponential decay (4.40). Finally we conclude (4.41) by inserting Lemma 4.2. \square

5. Numerical simulation

In the following we discuss the numerical simulation of the model (1.7), (1.8) in the film case.

5.1. Space discretization. The starting point of our approach is the weak formulation (2.13) and (2.14), to which we apply a finite element discretization in space. For this sake we assume that D is a rectangular domain and choose a triangular grid \mathcal{T}_h covering D and satisfying usual regularity conditions. Moreover, we use standard linear finite elements, i.e., functions in the discrete space

$$\mathcal{W}^h = \{ u \in C_{per}(D) \mid u|_T \text{ is affinely linear}, \forall T \in \mathcal{T}_h \}.$$

The semidiscretization of (2.13) and (2.14) consists in looking for functions $(\delta^h, u^h) \in C^1(0, T; \mathcal{W}^h)^2$ satisfying

$$\begin{aligned} \int_D \left[\frac{\partial \delta^h}{\partial t} \varphi Q^h + L \frac{\mathbf{P}^h \nabla \mu^h \cdot \nabla \varphi}{Q^h} + \delta^h \frac{\nabla u^h}{Q^h} \cdot \nabla \left(\frac{\partial u^h}{\partial t} \varphi \right) + \rho \frac{\partial u^h}{\partial t} \varphi \right] d\mathbf{x} \\ = \int_D [r_3 - \nabla u^h \cdot \mathbf{r}_{12}] \varphi d\mathbf{x} \end{aligned} \quad (5.1)$$

$$\begin{aligned} \int_D \left[b \frac{\partial u^h}{\partial t} \frac{w}{Q^h} + \psi(\delta^h) \frac{\nabla u^h \cdot \nabla w}{Q^h} - \delta^h \frac{\nabla u^h \cdot \nabla (w \mu^h)}{Q^h} - \rho w \mu^h \right] d\mathbf{x} \\ = 0 \end{aligned} \quad (5.2)$$

for all $(\varphi, w) \in \mathcal{W}^h$ and all $t \in (0, T)$, where $\mu^h = \psi'(\delta^h)$, $Q^h = \sqrt{1 + |\nabla u^h|^2}$, and $\mathbf{P}^h = (Q^h)^2 \mathbf{I} - \nabla u^h \otimes \nabla u^h$.

This system is supplemented by initial values

$$\delta^h(t=0) = \delta_0^h, \quad u^h(t=0) = u_0^h, \quad (5.3)$$

where $u_0^h \in \mathcal{W}^h$ and $\delta_0^h \in \mathcal{W}^h$ are discrete approximations of the initial values u_0 and δ_0 , e.g., the H^1 -projections to the subspace \mathcal{W}^h .

5.2. Time discretization. Now we turn our attention to the time discretization of (1.7), (1.8). Since the adatom surface diffusion model consists of second-order equations, an explicit time discretization seems unfavourable due to severe stability restrictions on the time step. On the other hand, a fully implicit discretization leads to strongly nonlinear equations in each time step, which may be difficult to solve. We therefore construct a semi-implicit scheme, which only needs the solution of linear equations in each time step.

Semi-implicit schemes for the original surface diffusion model have been introduced in [6], and analyzed in [18]. The approach for surface diffusion can serve as a guideline for the time discretization of some terms in (5.1), (5.2). For the additional nonlinear terms we propose to use a semi-discretization yielding symmetry of the discretized problem. If we decompose the time interval into $[0, T] = \cup_k (t_k, t_{k+1})$ with $t_k = k\tau = \frac{k}{N}T$, then we compute the values $u_k^h = u^h(t_k)$ and $\delta_k^h = \delta^h(t_k)$ from the semi-discrete time step

$$\begin{aligned} \int_D \left[D_\tau \delta_k^h \varphi Q_k^h + c^k L \frac{\mathbf{P}_k^h \nabla \delta_{k+1}^h \cdot \nabla \varphi}{Q_k^h} + \delta_k^h \frac{\nabla u_k^h}{Q_k^h} \cdot \nabla (D_\tau u_k^h \varphi) + \rho D_\tau u_k^h \varphi \right] d\mathbf{x} \\ = \int_D L \frac{\mathbf{P}_k^h \nabla (c^k \delta_k^h - \mu_k^h) \cdot \nabla \varphi}{Q_k^h} d\mathbf{x} + \int_D [r_3 - \nabla u_k^h \cdot \mathbf{r}_{12}] \varphi d\mathbf{x} \end{aligned} \quad (5.4)$$

$$\begin{aligned} \int_D \left[b D_\tau u_k^h \frac{w}{Q_k^h} + \psi(\delta_k^h) \frac{\nabla u_{k+1}^h \cdot \nabla w}{Q_k^h} - c^k \delta_k^h \frac{\nabla u_k^h \cdot \nabla (w \delta_{k+1}^h)}{Q_k^h} - \rho w c^k \delta_{k+1}^h \right] d\mathbf{x} \\ = - \int_D \left[\delta_k^h \frac{\nabla u_k^h \cdot \nabla (w (c^k \delta_k^h - \mu_k^h))}{Q_k^h} + \rho w (c^k \delta_k^h - \mu_k^h) \right] d\mathbf{x}, \end{aligned} \quad (5.5)$$

with $D_\tau u_k^h := \frac{u_{k+1}^h - u_k^h}{\tau}$, $\mu_k^h = \psi'(\delta_k^h)$ and $c^k > 0$ being a constant such that

$$c^k \geq \max_{\mathbf{x}} \psi''(\delta_k^h(\mathbf{x})).$$

In the case of the quadratic surface free energy (3.2) we can choose $c^k = \gamma$ and thus $\gamma \delta_k^h = \mu_k^h$ for all k .

5.3. Structure of discretized problems. The system (5.4), (5.5) can be rewritten as a linear system for the nodal values (Δ, U) of $(\delta_{k+1}^h, u_{k+1}^h)$. This yields

$$\begin{pmatrix} \tau^{-1}\mathbf{M}_1 + \mathbf{K}_1 & -\tau^{-1}\mathbf{L} \\ c_0\mathbf{L}^T & \tau^{-1}\mathbf{M}_2 + \mathbf{K}_2 \end{pmatrix} \begin{pmatrix} \Delta \\ U \end{pmatrix} = \begin{pmatrix} F \\ G \end{pmatrix}. \quad (5.6)$$

The matrices \mathbf{M}_1 and \mathbf{M}_2 are mass matrices, \mathbf{K}_1 and \mathbf{K}_2 are stiffness matrices, and \mathbf{L} is the only non-symmetric matrix, corresponding to the discretization of the sum of a first-order and a zero-order term.

We now multiply the first equation by $-\tau c_0$ and exchange the order of equations and variables in (5.6) to obtain the equivalent linear system

$$\begin{pmatrix} \tau^{-1}\mathbf{M}_2 + \mathbf{K}_2 & c_0\mathbf{L}^T \\ c_0\mathbf{L} & -c_0(\mathbf{M}_1 + \tau\mathbf{K}_1) \end{pmatrix} \begin{pmatrix} U \\ \Delta \end{pmatrix} = \begin{pmatrix} G \\ -c_0\tau F \end{pmatrix}. \quad (5.7)$$

We can now further introduce a dual variable P and equivalently rewrite the system (with the notation $\mathbf{A} = \tau^{-1}\mathbf{M}_2 + \mathbf{K}_2$ and $\mathbf{B} = c_0(\mathbf{M}_1 + \tau\mathbf{K}_1)$)

$$\begin{pmatrix} \mathbf{A} & 0 & c_0\mathbf{L}^T \\ 0 & \mathbf{B} & -\mathbf{B} \\ c_0\mathbf{L} & -\mathbf{B} & 0 \end{pmatrix} \begin{pmatrix} U \\ \Delta \\ P \end{pmatrix} = \begin{pmatrix} G \\ 0 \\ -c_0\tau F \end{pmatrix}. \quad (5.8)$$

The expanded problem (5.8) is the first-order optimality condition of the linearly constrained quadratic optimization problem

$$\frac{1}{2}U^T \mathbf{A}U + \frac{1}{2}\Delta^T \mathbf{B}\Delta - G^T U \rightarrow \min_{U, \Delta} \quad (5.9)$$

$$\text{subject to } c_0\mathbf{L}U - \mathbf{B}\Delta = -c_0\tau F, \quad (5.10)$$

and due to convexity, the optimization problem and the first-order optimality condition are equivalent. Since the objective function is bounded, coercive, and strictly convex, and since the admissible set is bounded and nonempty (which is easy to see by setting $U=0$ and solving for W), we obtain:

THEOREM 5.1. *There exists a unique solution of the fully discrete problem (5.4), (5.5), respectively of the equivalent linear system (5.6).*

The well-posedness result for the discrete problem provides no information about the conditioning of the linear system (5.6). For $d=1$, the system size is even for fine discretization sizes small enough that direct solvers can be used to obtain the solution with reasonable efficiency. For finer discretizations of surfaces ($d=2$) it may be advantageous to use an iterative solver, in particular if the time step is not too large and thus, the previous time step may provide a good initial value for the iteration. Since (5.6) respectively the symmetrized form (5.7) is indefinite, one cannot use standard iterations and preconditioners for second-order elliptic partial differential

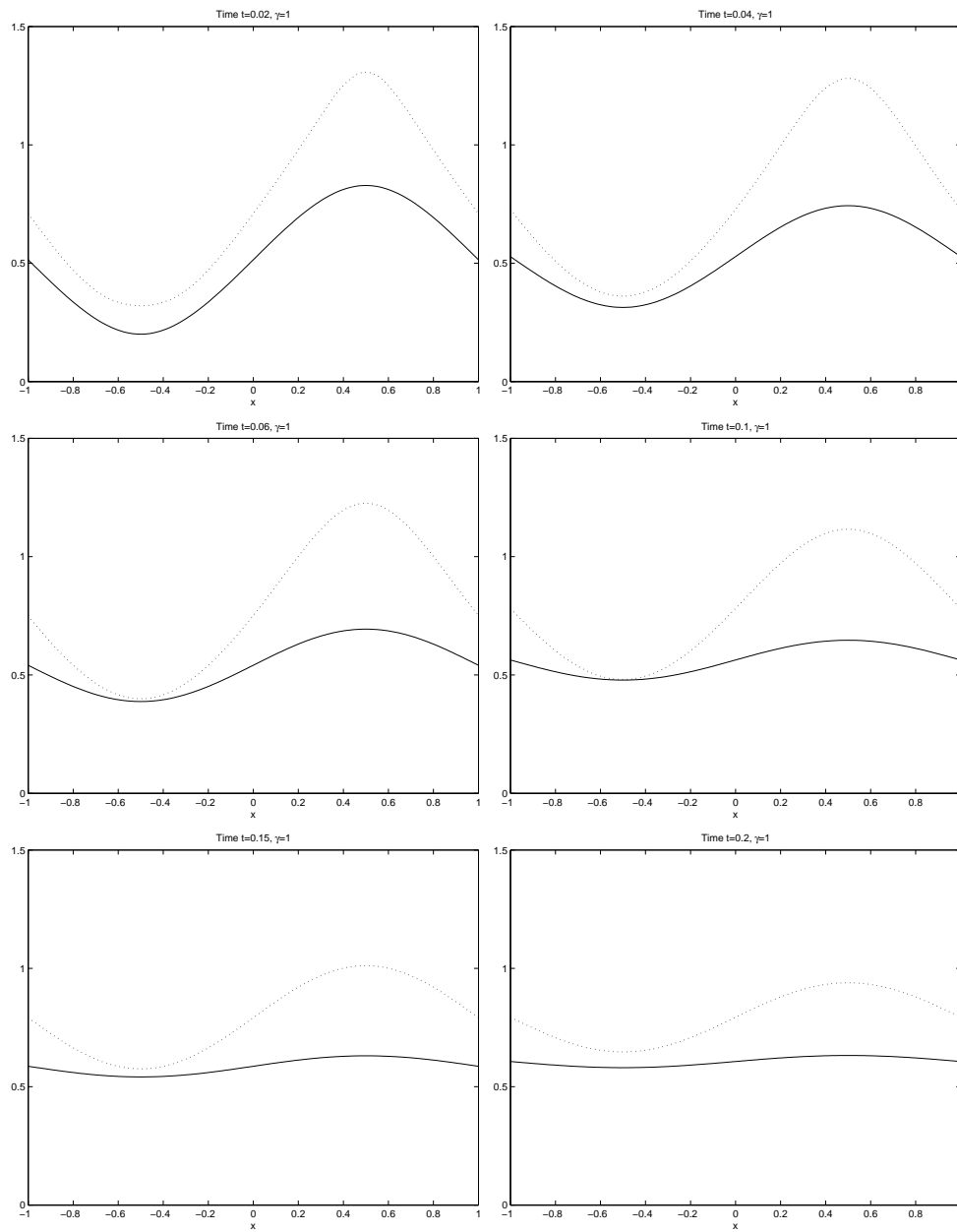


FIG. 5.1. Evolution for $\gamma=1$, $\delta^0 \equiv 0.2$, $u^0 = 0.5 + 0.5\sin(\pi x)$.

equations, but more general Krylov-subspace iterations such as GMRES or QMR (cf. [42]). As a simple approach for the preconditioning one can use block-diagonal matrices such as

$$\mathbf{P} = \begin{pmatrix} \tau^{-1}\hat{\mathbf{M}}_2 + \hat{\mathbf{K}}_2 & 0 \\ 0 & -c_0(\hat{\mathbf{M}}_1 + \tau\hat{\mathbf{K}}_1) \end{pmatrix}$$

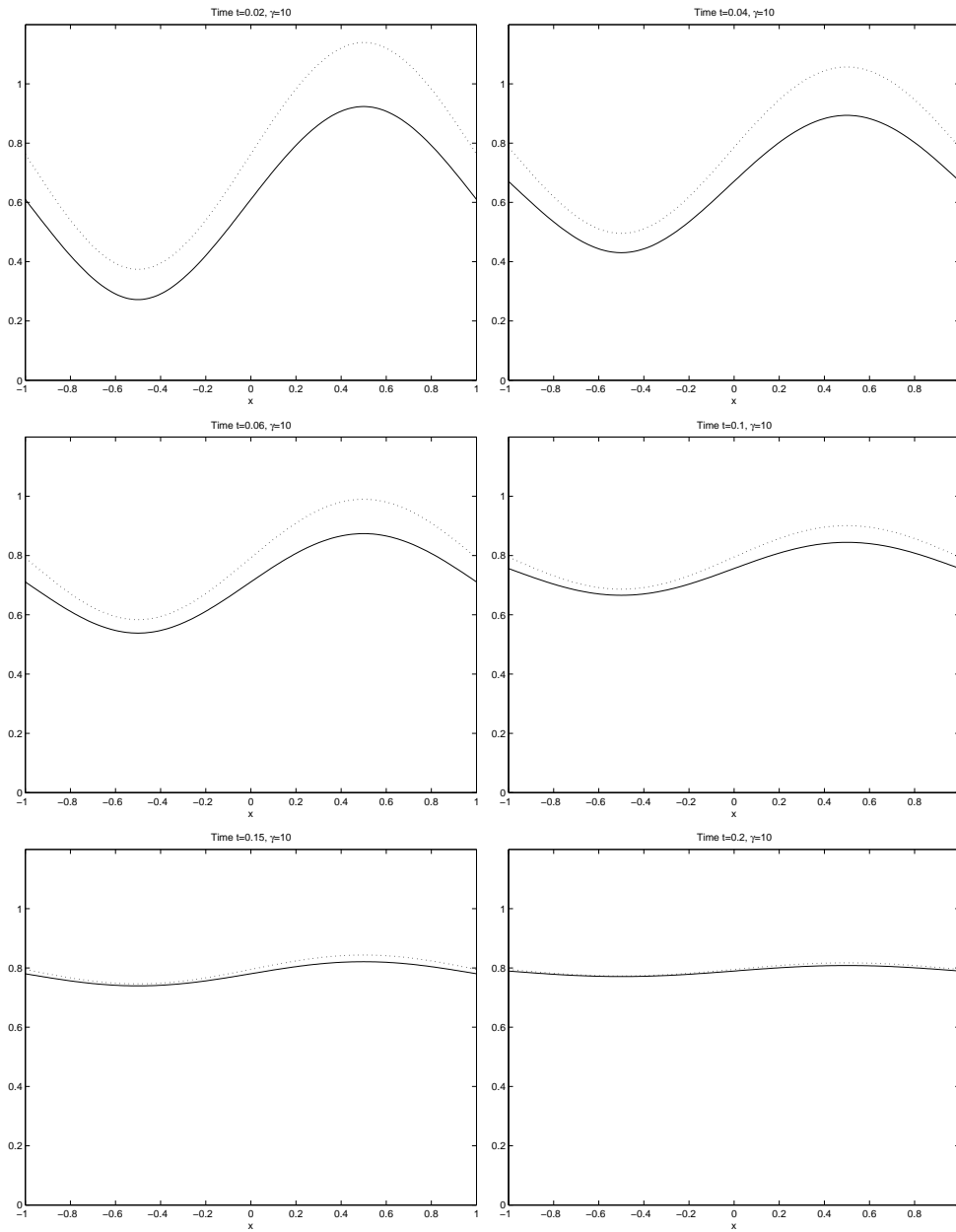


FIG. 5.2. Evolution for $\gamma=10$, $\delta^0 \equiv 0.2$, $u^0 = 0.5 + 0.5\sin(\pi x)$.

with standard preconditioners $\hat{\mathbf{M}}_i$ and $\hat{\mathbf{K}}_i$ for the mass and stiffness matrices. In our numerical tests, this yields reasonable results, but a more detailed investigation of suitable preconditioning strategies is definitely needed in future research, with the possible aim of performing large-scale simulations of thin films with nanoscale surface modulations.

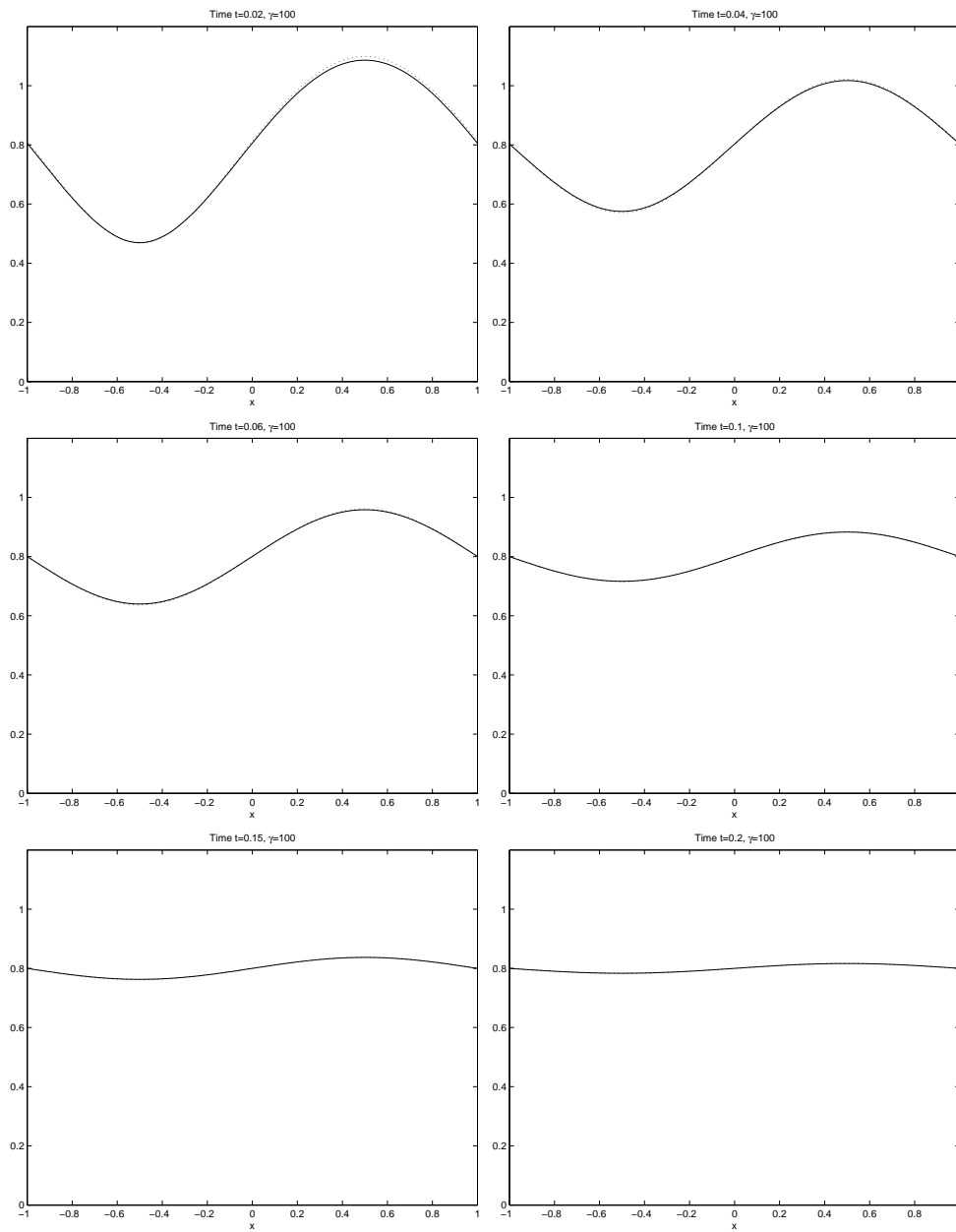


FIG. 5.3. Evolution for $\gamma = 100$, $\delta^0 \equiv 0.2$, $u^0 = 0.5 + 0.5\sin(\pi x)$.

5.4. Results.

We now present some simulation results obtained with the scheme discussed above. We start with planar curves, i.e., $d=1$, and use the domain $D=(-1,1)$. In this case we illustrate the results by plotting the curve shape as a solid line and the adatom density as a dotted graph over the surface.

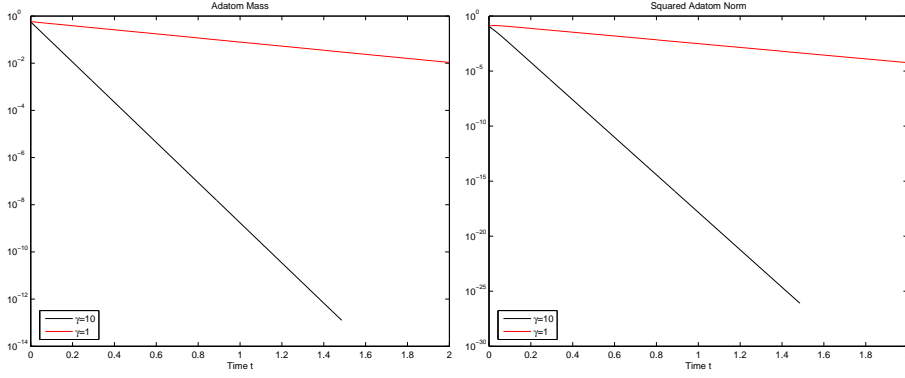


FIG. 5.4. Semilogarithmic plot of the adatom mass $\int_{\Gamma(t)} \delta(t) dS$ and of the squared norm $\int_{\Gamma(t)} \delta(t)^2 dS$ vs. time t (for $\gamma=1$ and $\gamma=10$).

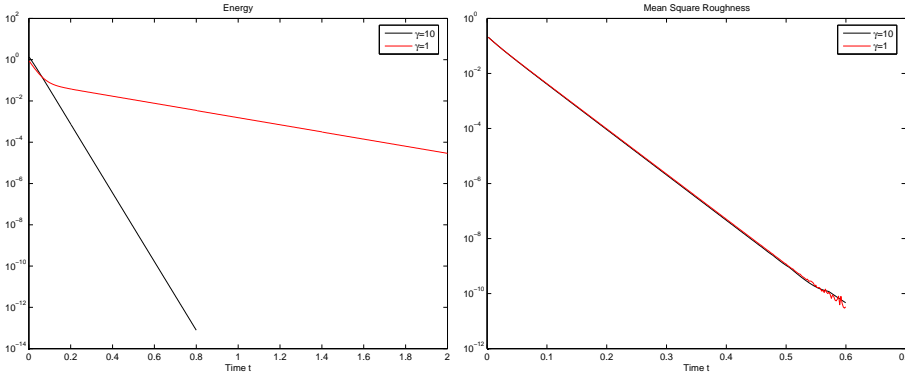


FIG. 5.5. Semilogarithmic plot of the energy difference $\int_{\Gamma(t)} \psi(\delta(t)) dS - 2$ and of the squared norm $\int_D (u(t) - \bar{u}(t))^2 dx$ vs. time t (for $\gamma=1$ and $\gamma=10$).

The first example uses an initial value far away from equilibrium given by

$$u^0(x) = 0.5 + 0.5 \sin(\pi x), \quad \delta^0 \equiv 0.2. \quad (5.11)$$

We study the evolution towards equilibrium for different values of γ in the surface free energy $\psi(\delta) = 1 + \frac{\gamma}{2} \delta^2$. The further parameters used are $b=0.5$, $L=1$. In Figures 5.1, 5.2, and 5.3 we show the results for the values $\gamma=1$, $\gamma=10$, and $\gamma=100$ at the time steps $t=0.02, 0.04, 0.06, 0.1, 0.15, 0.2$, computed with a time step $\tau=0.002$. One observes that for increasing γ , the adatom densities are decreasing towards zero, for $\gamma=100$ there are hardly free adatoms and the evolution is very close to the one obtained with the kinetic surface diffusion model (2.15), (2.16). In all three cases, the evolution of the free boundary shape Γ is very similar, while the decay of the adatom density is clearly much faster for large values of γ .

The long-time behaviour is illustrated in Figures 5.4 and 5.5. Figure 5.4 shows semilogarithmic plots of the adatom mass and the squared norm $\int_{\Gamma(t)} \delta(t)^2 dS$ vs. time. One observes that both decay to zero exponentially in time, a behaviour we

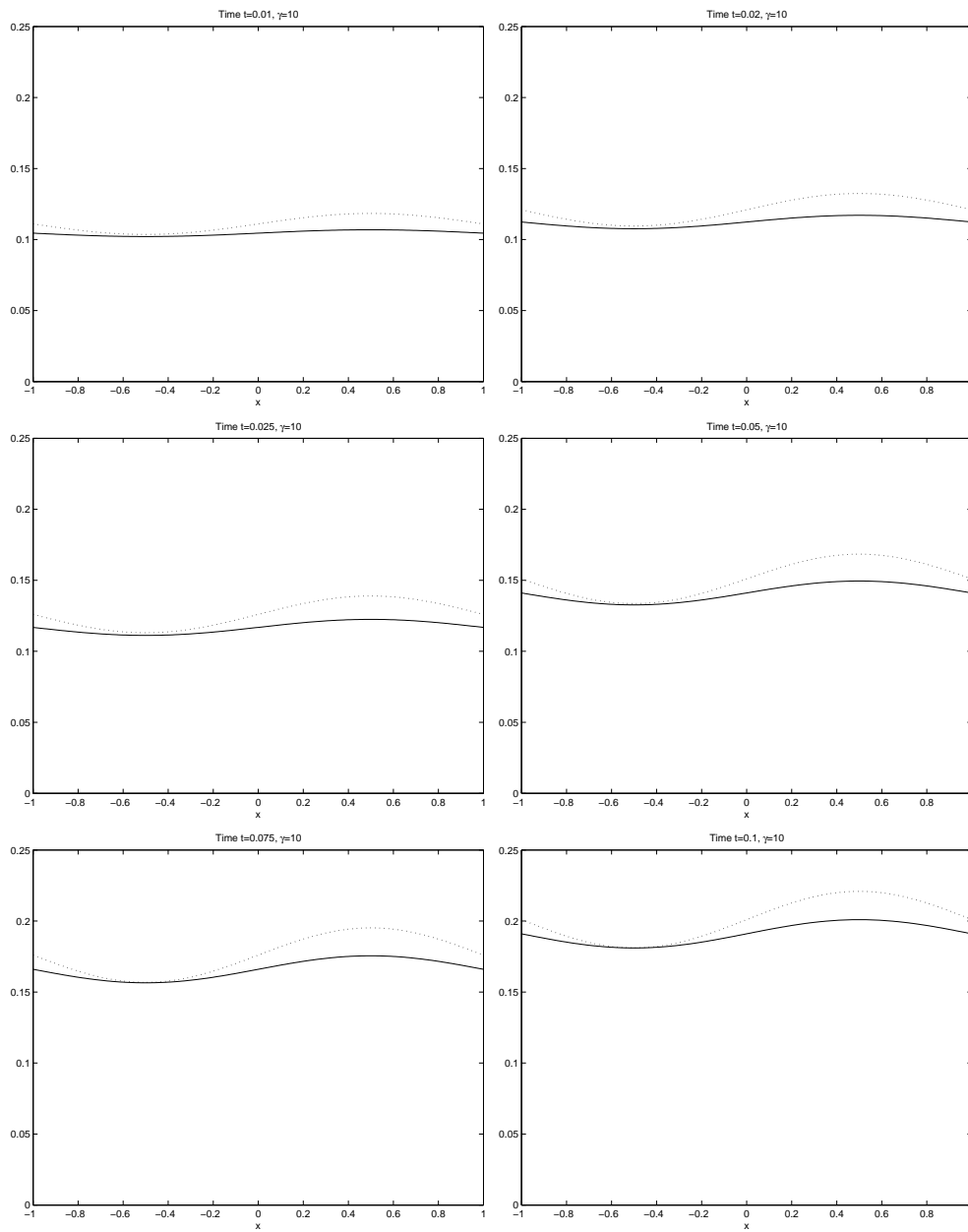


FIG. 5.6. Evolution for $\gamma=10$, $\delta^0 \equiv 0$, $u^0 = 0.1$, $r_3 = 1 + \sin(\pi x)$, $b = 0.1$.

observe in all experiments without deposition flux, thus confirming Theorem 4.5. Figure 5.5 shows semilogarithmic plots of the difference of the surface energy to the equilibrium value, i.e. $\int_{\Gamma(t)} \psi(\delta(t)) dS - 2$, and of the mean square roughness $\int_D (u(t) - \bar{u}(t))^2 dx$, where $\bar{u}(t)$ is the mean value of $u(t)$. One observes that also these two measures decay to zero exponentially in time, a behaviour that was also observed in the other numerical experiments.

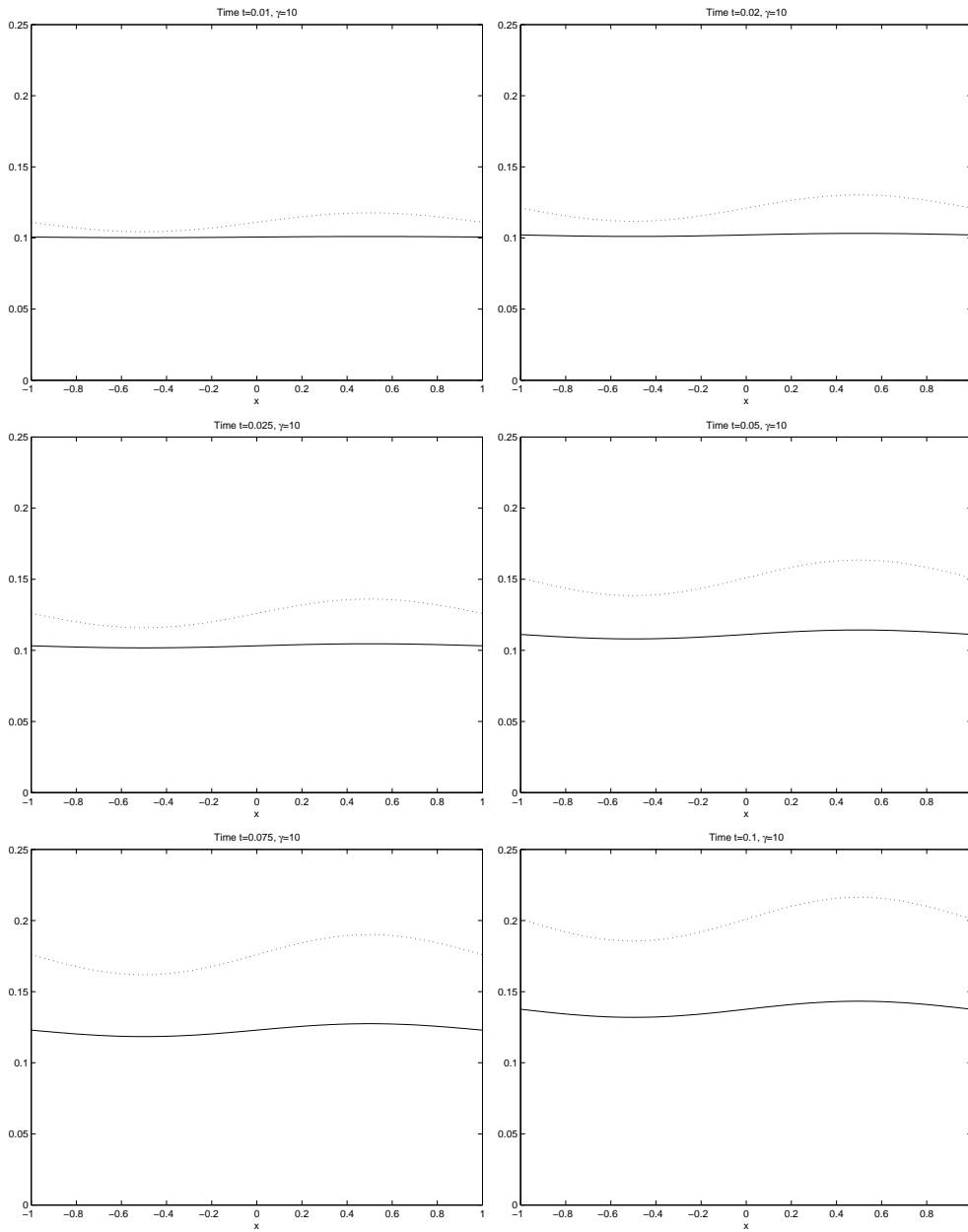


FIG. 5.7. Evolution for $\gamma=10$, $\delta^0 \equiv 0$, $u^0=0.1$, $r_3=1+\sin(\pi x)$, $b=1$.

The second experiment in the one-dimensional case corresponds to a typical situation appearing in practice: The initial value is a flat curve at equilibrium (and no free adatoms), and we start a heterogeneous deposition in a vertical direction for time $t > 0$, determined by the deposition rate $r_3 = 1 + \sin(\pi x)$. The results for two different values of the kinetic coefficient b are illustrated in Figures 5.7 ($b=0.1$) and 5.8 ($b=1$). One observes that for a small kinetic coefficient, the shape of the film

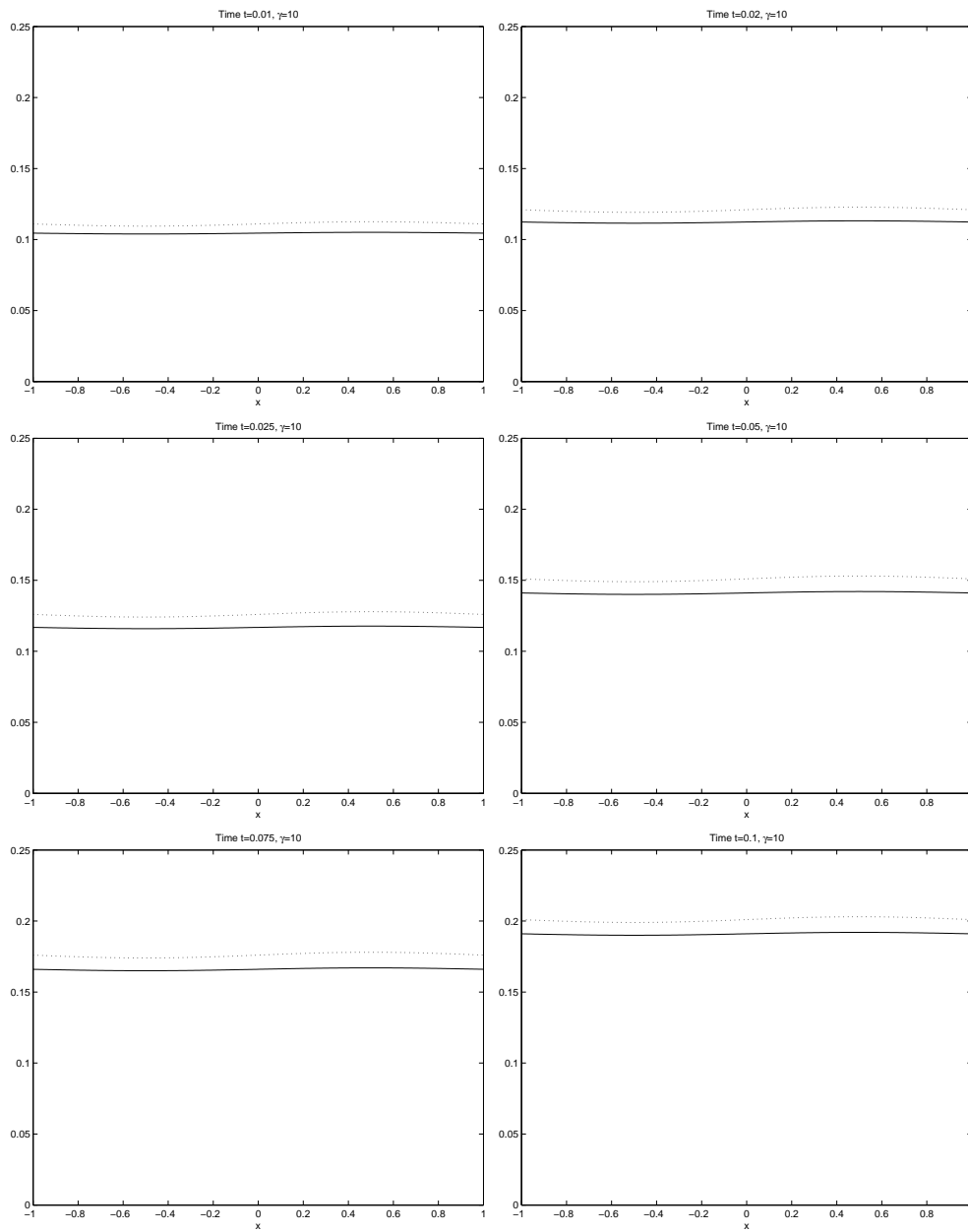


FIG. 5.8. Evolution for $\gamma = 10$, $(\delta^0, u^0) \equiv (0, 0.1)$, $r_3 = 1 + \sin(\pi x)$, $b = 0.1$.

surface follows the sinusoidal shape of the deposition rate, while for a larger kinetic coefficient, the surface stays much closer to a flat shape, which numerically confirms the stabilizing effect of the kinetic term on the surface shape as conjectured in [26]. Figure 5.6 shows the evolution for a large value of γ , where the evolution is very close to the kinetic surface diffusion model. The computations illustrated in Figures 5.6–5.8 were performed with a time step $\tau = 0.001$.

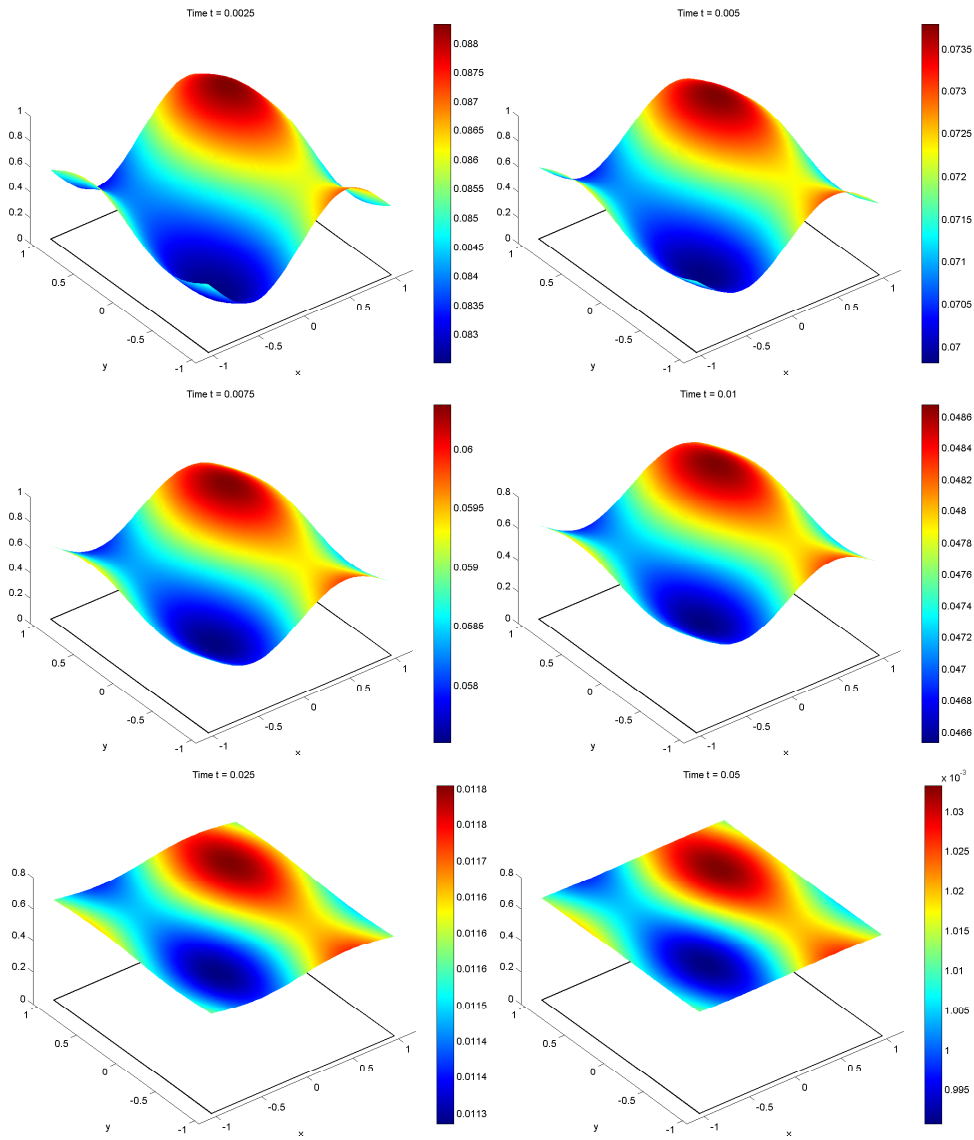


FIG. 5.9. Evolution for initial value $u^0 = 0.5 + 0.3\sin(\pi x) + 0.2\sin(\pi y)$, $\delta^0 \equiv 0.1$.

A general observation, which applies to all of the numerical experiments, is that adatom densities are usually higher where the mean curvature is negative, while the adatom density seems to attain its minimum over the surface where the mean curvature attains its maximum.

We also carried out a variety of two-dimensional simulations yielding qualitatively similar results as the one-dimensional films shown above. For this sake we only provide the results of two simulations here, which illustrate a peculiar multi-dimensional effect, namely a possibly different directional behaviour due to different scales appearing in the initial surface. For this simulation we use the parameters $L=0.1$, $\rho=1$, $b=0.1$,

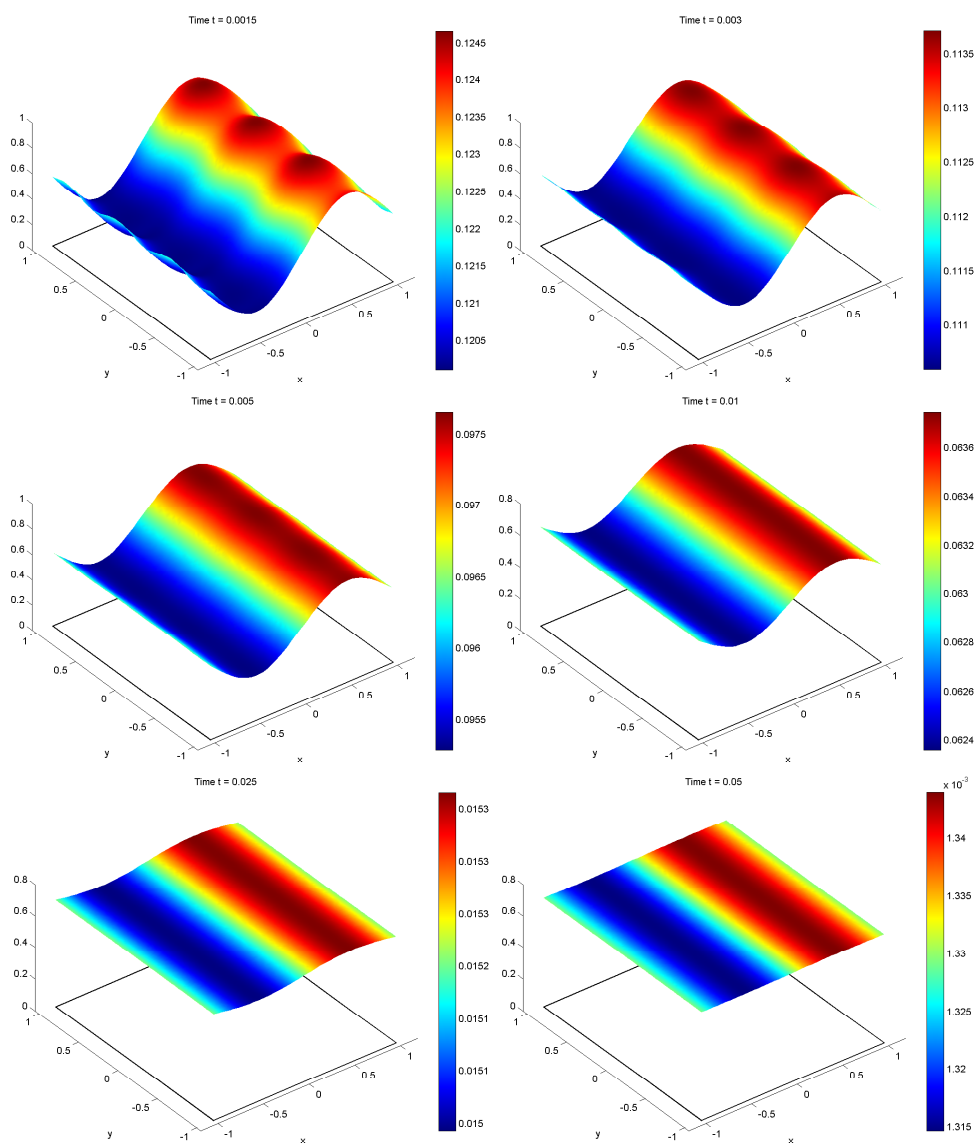


FIG. 5.10. Evolution for initial value $u^0 = 0.5 + 0.3\sin(\pi x) + 0.2\sin(3\pi y)$, $\delta^0 \equiv 0.1$.

$\gamma = 10$, $\mathbf{r} \equiv 0$, the time step $\tau = 5 * 10^{-4}$, and the computational domain $D = (-1, 1)^2$. The initial value for the adatom density is given by $\delta^0 \equiv 0.1$, and the one for the surface height by

$$u^0 = 0.5 + 0.3\sin(\pi x) + 0.2\sin(\pi y).$$

The resulting evolution is illustrated in Figure 5.9 at six different time steps. The plots show the graph of the surface height combined with color plots of the adatom densities on the surfaces. One observes again that adatom densities are lower in convex regions of the surface than in concave regions, but there is no unique trend around

saddle points, where nonlocal effects may play a larger role. During the evolution, the surface becomes flat and the adatom density decreases to zero, which confirms the expected trend to equilibrium. Since the initial values have roughly the same scales in the x - and y -direction, the speed of the equilibration is roughly the same in both directions.

The situation changes by using a different initial value for the surface height,

$$u^0 = 0.5 + 0.3\sin(\pi x) + 0.2\sin(3\pi y),$$

where smaller scales appear in the y -direction. From the plots of the evolving surface and adatom densities in Figure 5.10 (now at even smaller time steps) one observes that the equilibration is much faster for the smaller scales, and after a certain time the surface morphology and adatom density show almost no variation in the y -direction. In a larger time scale, the surface tends to a flat shape and the adatom density decreases to zero like in a one-dimensional evolution.

6. Conclusions

We have investigated a recently proposed model for surface diffusion including free adatoms by analytical and numerical methods. From the analysis of the equilibrium problem and the structure of the energy functional it turns out that there are two distinct regimes, namely a stable one close to flat or spherical surfaces with small adatom densities and an unstable one for rough surfaces and large adatom densities. Moreover, we found that at equilibrium, the adatom density vanishes in the film case, but not for a closed curve or surface.

In the stable regime, we were able to obtain local existence results for the dynamics by surface diffusion, and we derived local expansions around flat and spherical surfaces, which provide a further insight into the cross-diffusion structure of the model. One observes that the first-order expansion has a backward-diffusion term if the condition (4.12), which can be interpreted as a smallness condition on the adatom density, is violated. On the other hand, we obtain existence close to flat and spherical shapes and linear stability of equilibria. Moreover, for smooth solutions the energy and adatom density decay exponentially. Hence, the different behaviour in two regimes appears in the dynamics, too. A more detailed investigation of the unstable regime and stabilizing effects like curvature regularization in the dynamics is left open as a challenging topic for future research.

Finally, we also provided numerical simulations based on finite element discretizations and semi-implicit time stepping. The detailed numerical analysis of the algorithm as well as numerical methods for more complicated situations is beyond the scope of this paper, but provides an important subject for future investigations.

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