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Island Dynamics Models for Molecular Beam Epitaxy: Stability Analysis and Model Reduction *

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Abstract

We consider two island dynamics models recently developed for crystal growth by molecular beam epitaxy: the irreversible aggregation model and the attachment-detachment model. We examine the well-posedness of these continuum models and the linear stability of step edges in step-flow growth. We also present some reduced attachment-detachment models that can be used for analysis and simulation.

Keywords: molecular beam epitaxy, island dynamics, diffusion, linear stability, model reduction.

AMS Mathematics Subject Classification: 35Q99, 35R35.

1 Introduction

A class of island dynamics models have been recently developed for the growth of semiconductor thin films by molecular beam epitaxy [4, 5, 11, 12]. These models describe the motion of boundaries of adatom islands as well as the distribution of adatom density. A distinguished feature of these models is that they remain continuum in the lateral spatial directions and time, but discrete in the growth direction. Such a model consists of a diffusion equation for the adatom density and an evolution equation for the island boundaries. Numerical solution of these differential equations has been performed in order to simulate thin film growth [5, 8, 11, 12].

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We are interested in two island dynamics models. The first one is called the "irreversible aggregation" model. The corresponding boundary condition (on island boundaries) is that the adatom density vanishes on boundaries of islands, which follows from the assumption that an adatom sticks irreversibly to a boundary immediately after it hits the boundary. The second model is called the "attachment-detachment" model. It involves not only the island boundaries and the adatom density but also the density of edge adatoms — atoms that diffuse along island boundaries — and the density of kinks along island boundaries. Both the attachment and detachment of adatoms to and from the boundaries are described in the model. The underlying continuum equations include the diffusion equation for the adatom density together with a mixed type boundary condition, the diffusion equation for the edge adatom density, and the convection equation for the kink density. In this work, we apply these models to study the morphology of a periodic sequence of step edges in step-flow epitaxial growth of a thin film. Our goal is to understand the mathematical well-posedness of these models and to use these models to predict the linear stability of a step edge in step-flow growth. We also propose some reduced attachment-detachment models that can be used for simulation and analysis.

Our method for analyzing the linear stability is standard: we first find a steady-state solution of the underlying system; we then linearize the system around such a solution; we further obtain the dispersion relation from the solutions of the linearized system; and we finally use the dispersion relation to analyze the asymptotic behavior of the frequency for small and large wave numbers. We find that the irreversible aggregation model is mathematically ill-posed and that dendritic instability can occur, with a growth rate of order $O(l)$, for large wave numbers l. But the instability is weak, since the coefficient of the growth rate is small due to two-sided attachment. For the attachment-detachment model, we only consider the steady and quasi-steady systems, which is justified by the large magnitude of adatom diffusion constants for most practical applications. We find for practically allowable parameters that both systems are asymptotically stable. Moreover, the frequency is proportional to $O\left(l^2\right)$ for both small and large wave numbers l. The constants of proportion are solely characterized by the edge Péclet number, an input parameter which is proportional to both the constant deposition flux rate and the step width but inversely proportional to the edge adatom diffusion constant. In fact, for small edge Péclet numbers, both systems are stable for any wave numbers. Note that the Mullins-Sekerka type instability of a step edge (cf. [1, 6, 9, 10]) is excluded in this model due to the edge adatom diffusion and kink convection.

For numerical simulation, we propose a simpler attachment-detachment model by dropping the spatial and temporal derivative terms in the equations of edge adatom diffusion and kink convection. For better understanding the role of edge adatom diffusion and kink convection, we propose a reduced model that only involves edge adatom density and kink density but not the adatom density. We find that the dispersion relation for the original attachment-detachment model is qualitatively recaptured by our reduced models.

Section 2 describes the two island dynamics models. Stability analysis for the irreversible aggregation model is presented in Section 3. In Section 4, we analyze the linear

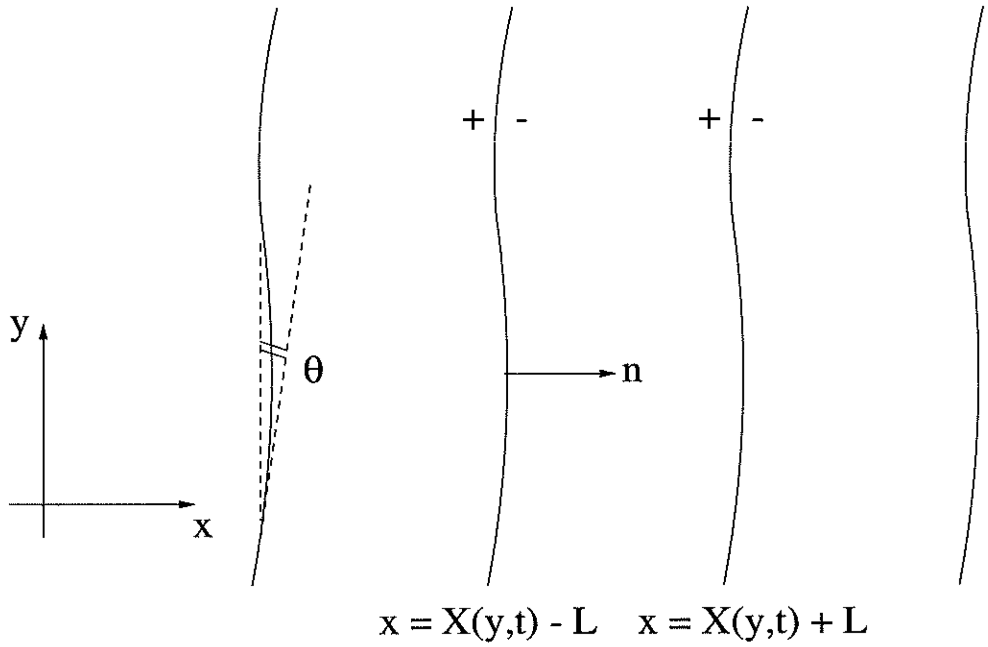

Figure 2.1. The geometry of step-flow growth of a crystal.

stability for both the quasi-steady and steady systems for the attachment-detachment model. In Section 5, we propose several reduced models, study their linear stabilities, and compare them with those of the original attachment-detachment model.

2 Island dynamics models

We briefly describe the two island dynamics models applied to step-flow growth of a thin film by molecular beam epitaxy. See [4, 5] for detailed derivation of these models.

Consider a simple cubic crystal with lattice spacing a and two of its crystallographic directions parallel to Ox and Oy axes, respectively. The geometry of step-flow growth of the crystal consists of a sequence of periodical steps that move as time t increases. See Figure 2.1. Each step is of one atomic layer lower than its preceding one. Edges of these steps are nearly flat and almost parallel to one of the crystallographic directions, say, the Oy axis. We represent these step edges by functions

$$x = X(y,t) + (2j+1)L, \qquad j = 0, \pm 1, \cdots,$$

where $X(y,t)$ is a smooth function and $L > 0$ is half of the step width. For each point (x, y) on a step edge, we denote by $\theta = \theta(y,t)$ the signed angle between the tangent of the step edge and Oy axis,

$$\tan\theta = -\partial_y X, \qquad -\pi/2 < \theta < \pi/2. \tag{2.1}$$

The curvature $\kappa = \kappa(y,t)$, the unit normal $\mathbf{n} = \mathbf{n}(y,t)$ pointing from the upper (marked by +) into lower (marked by −) terrace, and the normal velocity $v = v(y,t)$ of the step edge are given respectively by

$$\kappa = \partial_s \theta, \qquad \mathbf{n} = (\cos\theta, \sin\theta), \qquad v = \partial_t X \cos\theta, \tag{2.2}$$

where ∂_s is the tangential derivative in the y direction. By (2.1) and (2.2), we have

$$\mathbf{n} = \frac{1}{\sqrt{1+(\partial_y X)^2}}(1, -\partial_y X) \quad \text{and} \quad v = \frac{\partial_t X}{\sqrt{1+(\partial_y X)^2}}. \tag{2.3}$$

Note that the sign of θ has been changed from that used in [4]. This avoids a minus sign in the definition of curvature κ.

2.1 The irreversible aggregation model

This model involves the step edge function $x = X(y,t)$ and the adatom density $\rho = \rho(x,y,t)$, which is assumed to be periodic in x with periodicity $2L$. The model consists of the adatom diffusion equation on the steps together with boundary conditions and jump conditions along step edges. On a typical step defined by $X(y,t) - L < x < X(y,t) + L$, these equations and side conditions are

$$\partial_t \rho - D\nabla^2 \rho = F \qquad \text{for } X(y,t) - L < x < X(y,t) + L, \tag{2.4}$$

$$\rho = 0 \qquad \text{at } x = X(y,t) \pm L, \tag{2.5}$$

$$D\mathbf{n} \cdot [\nabla \rho] = -a^{-2} v, \tag{2.6}$$

where D is the adatom diffusion constant, F is the constant deposition flux rate, $[u]$ denotes the jump for a function u defined by $[u] = u_+ - u_-$ with $u_\pm$ the restriction of u on the edge $X \pm L$, $\mathbf{n}$ is the unit normal to the edge given in (2.3), and v is the normal velocity also given in (2.3).

2.2 The attachment-detachment model

Besides the step edges represented by $x = X(y,t)$, there are three physical quantities in this model. They are the adatom density $\rho = \rho(x,y,t)$ defined on steps, the edge adatom density $\phi = \phi(y,t)$ defined on all step edges, and the kink density $k = k(y,t)$ also defined on all step edges. The function $\rho = \rho(x,y,t)$ is periodical in the variable x with periodicity $2L$. Introducing the density of right-facing (or up-facing) kinks $k_r = k_r(y,t)$ and that of left-facing (or down-facing) kinks $k_l = k_l(y,t)$, we assume that

$$\begin{aligned} k_r + k_l &= k, \\ k_r - k_l &= a^{-1} \tan\theta. \end{aligned} \tag{2.7}$$

The attachment-detachment model consists of a set of evolutionary equations together with boundary conditions and a set of constitutive relations. On a typical step defined by $X(y,t) - L < x < X(y,t) + L$, these equations and boundary conditions are

$$\partial_t \rho - D\nabla^2 \rho = F \qquad \text{for } X(y,t) - L < x < X(y,t) + L, \tag{2.8}$$

$$v\rho_+ + D\mathbf{n} \cdot \nabla \rho_+ = -f_+ \qquad \text{at } x = X(y,t) + L, \tag{2.9}$$

$$v\rho_- + D\mathbf{n} \cdot \nabla \rho_- = f_- \qquad \text{at } x = X(y,t) - L, \tag{2.10}$$

$$\partial_t \phi - d\partial_s^2 \phi = f_+ + f_- - f_0, \tag{2.11}$$

$$\partial_t k + \partial_s (w(k_r - k_l)) = 2(g - h). \tag{2.12}$$

Here, Eq. (2.8) describes the adatom diffusion on terraces, in which D is the adatom diffusion constant and F is the constant deposition flux rate. Eqs. (2.9) and (2.10) are the boundary conditions for the adatom density ρ, in which ρ_+ and ρ_- are the restrictions to the step edge from upper and lower terraces, respectively, and $f_+ = f_+(y,t)$ and $f_- = f_-(y,t)$ are the net fluxes to the step edge from upper and lower terraces, respectively. Eq. (2.11) describes the diffusion of edge adatoms along step edges, in which d is the edge adatom diffusion constant and $f_0 = f_0(y,t)$ is the net loss term due to attachment of edge adatoms to kinks. Eq. (2.12) describes the convection of kinks, in which, $w = w(y,t)$ is the kink velocity, and $g = g(y,t)$ and $h = h(y,t)$ represent, respectively, the creation and annihilation of left-right kink pairs. Notice that left-facing kinks and right-facing kinks move in opposite directions with velocity w and $-w$, respectively.

The quantities $f_\pm$, f_0, w, g, h, and v are determined by the following constitutive relations

$$f_+ = \alpha a \rho_+ - \beta\phi, \tag{2.13}$$

$$f_- = \alpha a \rho_- - \beta\phi, \tag{2.14}$$

$$f_0 = v\left(\phi\kappa + a^{-2}\right), \tag{2.15}$$

$$w = a^2\left[l_1\beta\phi + \alpha a(l_2\rho_+ + l_3\rho_-)\right], \tag{2.16}$$

$$g = a\phi\left[m_1\beta\phi + \alpha a(m_2\rho_+ + m_3\rho_-)\right], \tag{2.17}$$

$$h = a^2 k_r k_l\left[n_1\beta\phi + \alpha a(n_2\rho_+ + n_3\rho_-)\right], \tag{2.18}$$

$$v = awk\cos\theta, \tag{2.19}$$

where $\alpha = a^{-2}D$ is the hopping rate of an adatom on a terrace, $\beta = a^{-2}d$ is the hopping rate of an edge adatom along or off an edge, and all l_i, m_i, n_i $(i = 1,2,3)$ are positive (but not necessary integer) parameters. (Note that the notation n_1 is used here for a constant parameter in (2.18). It is neither the first component nor the first order perturbation of the unit normal $\mathbf{n}$.) The relations (2.13), (2.14), and (2.16) – (2.18) are determined by a mean field theory [3, 4], (2.15) is derived from the conservation of mass [4], and (2.19) is a generalization of the classical Burton-Cabrera-Frank theory [2, 7].

Note that for simplicity, a number of physical effects have been neglected. They include desorption of adatoms into vapor, nucleation of islands on steps, and step-edge asymmetry. Note also that in [4], the parameters are fixed to be $(l_1, l_2, l_3) = (2, 2, 1)$, $(m_1, m_2, m_3) = (2, 4, 2)$, and $(n_1, n_2, n_3) = (2, 3, 1)$.

3 Stability for the irreversible aggregation model

Let us first find a steady-state solution for the system (2.4) – (2.6). To do so, we consider flat step edges determined by $X_0(y,t) = v_0 t$ with $v_0 > 0$ the constant normal velocity. The corresponding unit normal of the step edge is $\mathbf{n}_0 = (1, 0)$. We seek $\rho_0 = \rho_0(x, y, t)$ that satisfies (2.4) – (2.6) with X and ρ replaced by X_0 and ρ_0, respectively. By the change of variable $\tilde{x} = x - v_0 t$, we obtain for $\tilde{\rho}_0(\tilde{x}, y, t) = \rho_0(x, y, t)$ that

$$
\begin{aligned}
\partial_t \tilde{\rho}_0 - v_0 \partial_{\tilde{x}} \tilde{\rho}_0 - D\nabla^2 \tilde{\rho}_0 = F \qquad & \text{for } -L < \tilde{x} < L, \\
\tilde{\rho}_0 = 0 \qquad & \text{at } \tilde{x} = \pm L, \\
D \left[\partial_{\tilde{x}} \tilde{\rho}_0 \right] = -a^{-2} v_0, &
\end{aligned}
$$

where the jump $[\cdot]$ is defined by the limiting values at $\tilde{x} = \pm L$. Assume that $\tilde{\rho}_0$ is independent of y and t. Then, we can solve the above system to get

$$
v_0 = 2a^2 FL \quad \text{and} \quad \tilde{\rho}_0 = b_0 + b_1 \tilde{x} + b_2 e^{-\lambda \tilde{x}}, \tag{3.1}
$$

where

$$
\lambda = D^{-1} v_0, \quad b_0 = \left(2a^2\right)^{-1} \coth(\lambda L), \quad b_1 = -\left(2a^2 L\right)^{-1}, \quad b_2 = -\left(2a^2 \sinh(\lambda L)\right)^{-1}.
$$

To derive the linearized system around the steady-state solution (3.1), we set

$$
X = X_0 + \epsilon X_1, \quad \rho = \rho_0 + \epsilon \rho_1, \quad \mathbf{n} = \mathbf{n}_0 + \epsilon \mathbf{n}_1, \quad v = v_0 + \epsilon v_1.
$$

From (2.3), we get that $\mathbf{n}_1 = (0, -\partial_y X_1)$ and $v_1 = \partial_t X_1$. Inserting the expansions for X and ρ into the system (2.4) — (2.6), using the solution (3.1), and comparing the terms of order $O(\epsilon)$, we obtain by a series of calculations the linearized system

$$
\begin{aligned}
\partial_t \rho_1 - D\nabla^2 \rho_1 = 0 \qquad & \text{for } v_0 t - L < x < v_0 t + L, \\
\rho_1 + X_1 \partial_x \rho_0 = 0 \qquad & \text{at } x = v_0 t \pm L, \\
D \left[\partial_x \rho_1 \right] + D X_1 \left[\partial_x^2 \rho_0 \right] = -a^{-2} \partial_t X_1, &
\end{aligned}
$$

where the jumps are defined using the limiting values at $v_0 t \pm L$. With the change of variables $\tilde{x} = x - v_0 t$ and $\tilde{\rho}_1(\tilde{x}, y, t) = \rho_1(x, y, t)$, this system is equivalent to

$$
\begin{aligned}
\partial_t \tilde{\rho}_1 - v_0 \partial_{\tilde{x}} \tilde{\rho}_1 - D\nabla^2 \tilde{\rho}_1 = 0 \qquad & \text{for } -L < \tilde{x} < L, \\
\tilde{\rho}_1 + X_1 \tilde{\rho}_0' = 0 \qquad & \text{at } \tilde{x} = \pm L, \\
D \left[\partial_{\tilde{x}} \tilde{\rho}_1 \right] + D X_1 \left[\tilde{\rho}_0'' \right] = -a^{-2} \partial_t X_1, &
\end{aligned} \tag{3.2}
$$

where $'$ denotes the derivative with respect to $\tilde{x}$ and the jumps are defined using the limiting values at $\pm L$.

To find the dispersion relation, assume that $\tilde{\rho}_1$ and X_1 are periodic with respect to y with periodicity p. Then, we can find solutions of the above linearized system (3.2) as follows

$$\tilde{\rho}_1 = \left(\hat{\rho}_+ e^{\hat{\alpha}_+ \tilde{x}} + \hat{\rho}_- e^{\hat{\alpha}_- \tilde{x}}\right) e^{\omega t + ily},$$
$$X_1 = \hat{X}_1 e^{\omega t + ily},$$

where $pl/2\pi$ is an integer and all $\hat{\rho}_\pm$, $\hat{\alpha}_\pm$, $\hat{X}_1$, and ω are constants. Insert the expression of $\tilde{\rho}_1$ into the first equation in (3.2) and use the solution (3.1), to obtain

$$D\hat{\alpha}_+^2 + v_0\hat{\alpha}_+ - \left(\omega + Dl^2\right) = 0, \tag{3.3}$$
$$D\hat{\alpha}_-^2 + v_0\hat{\alpha}_- - \left(\omega + Dl^2\right) = 0. \tag{3.4}$$

Moreover, from the second and third equations in (3.2), it follows that

$$\hat{\rho}_+ e^{\hat{\alpha}_+ L} + \hat{\rho}_- e^{\hat{\alpha}_- L} + \hat{X}_1 \tilde{\rho}_0'(L) = 0,$$
$$\hat{\rho}_+ e^{-\hat{\alpha}_+ L} + \hat{\rho}_- e^{-\hat{\alpha}_- L} + \hat{X}_1 \tilde{\rho}_0'(-L) = 0,$$
$$2D\left[\hat{\alpha}_+\hat{\rho}_+ \sinh(\hat{\alpha}_+ L) + \hat{\alpha}_-\hat{\rho}_- \sinh(\hat{\alpha}_- L)\right] + D\hat{X}_1\left[\tilde{\rho}_0''(L) - \tilde{\rho}_0''(-L)\right] = -a^{-2}\omega\hat{X}_1.$$

Hence, there exist nontrivial solutions $\tilde{\rho}_1$ and X_1 in the given forms if and only if the coefficient matrix of the above system of linear equations for $\hat{\rho}_+$, $\hat{\rho}_-$ and $\hat{X}_1$ is zero, i.e.,

$$\begin{vmatrix} e^{\hat{\alpha}_+ L} & e^{\hat{\alpha}_- L} & \tilde{\rho}_0'(L) \\ e^{-\hat{\alpha}_+ L} & e^{-\hat{\alpha}_- L} & \tilde{\rho}_0'(-L) \\ 2D\hat{\alpha}_+ \sinh(\hat{\alpha}_+ L) & 2D\hat{\alpha}_- \sinh(\hat{\alpha}_- L) & D\left[\tilde{\rho}_0''(L) - \tilde{\rho}_0''(-L)\right] + a^{-2}\omega \end{vmatrix} = 0.$$

By a simple calculation, this leads to

$$\begin{aligned} &\left[\coth(\hat{\alpha}_+ L) - \coth(\hat{\alpha}_- L)\right]\left\{D\left[\tilde{\rho}_0''(L) - \tilde{\rho}_0''(-L)\right] + a^{-2}\omega\right\} + D\left(\hat{\alpha}_- - \hat{\alpha}_+\right) \\ &\quad \cdot \left[\tilde{\rho}_0'(L) + \tilde{\rho}_0'(-L)\right] + D\left[\tilde{\rho}_0'(L) - \tilde{\rho}_0'(-L)\right]\left[\hat{\alpha}_+ \coth(\hat{\alpha}_- L) - \hat{\alpha}_- \coth(\hat{\alpha}_+ L)\right] = 0. \end{aligned} \tag{3.5}$$

The three equations (3.3) – (3.5) determine $\hat{\alpha}_+ = \hat{\alpha}_+(l)$, $\hat{\alpha}_- = \hat{\alpha}_-(l)$, and $\omega = \omega(l)$ for each wave number l.

Proposition 3.1 *For the the irreversible aggregation model, the growth rate ω satisfies*

$$\omega(l) = \omega_0|l| + o(|l|) \qquad \textit{as } |l| \to \infty, \tag{3.6}$$

where

$$\omega_0 = a^2 D\left[\tilde{\rho}_0'(L) + \tilde{\rho}_0'(-L)\right] > 0.$$

Proof Observe from (3.5) that ω is of order not greater than $O(\hat{\alpha}_\pm)$. But by (3.3) and (3.4), $\hat{\alpha}_+$ and $\hat{\alpha}_-$ are the two roots of the same quadratic equation. Hence,

$$\hat{\alpha}_+ + \hat{\alpha}_- = -\frac{v_0}{D} \qquad \text{and} \qquad \hat{\alpha}_+\hat{\alpha}_- = -\frac{\omega + Dl^2}{D}.$$

It follows that $\hat{\alpha}_+$ and $\hat{\alpha}_-$ have the leading order terms $|l|$ and $-|l|$, respectively. Then, from the leading order terms in (3.5), we obtain the desired asymptotic expansion (3.6) by a series of calculations. By (3.1), we can verify that (since $\lambda L > 0$)

$$\tilde{\rho}_0'(L) + \tilde{\rho}_0'(-L) = \frac{\lambda L \cosh(\lambda L) - \sinh(\lambda L)}{a^2 L \sinh(\lambda L)} > 0.$$

The proof is complete. *Q.E.D.*

4 Stability for the attachment-detachment model

In this section, we consider the quasi-steady system obtained from the original system by replacing the diffusion equation (2.8) and the corresponding boundary conditions (2.9) and (2.10) in the attachment-detachment model by

$$-D\nabla^2\rho = F \qquad \text{for } X(y,t) - L < x < X(y,t) + L, \tag{4.1}$$

$$D\mathbf{n}\cdot\nabla\rho_+ = -f_+ \qquad \text{at } x = X(y,t) + L, \tag{4.2}$$

$$D\mathbf{n}\cdot\nabla\rho_- = f_- \qquad \text{at } x = X(y,t) - L, \tag{4.3}$$

respectively. We also consider the steady system consists of the above Eqs. (4.1) – (4.3) and the steady equations

$$-d\partial_s^2\phi = f_+ + f_- - f_0, \tag{4.4}$$

$$\partial_s(w(k_r - k_l)) = 2(g - h), \tag{4.5}$$

together with the constitutive relations (2.13) – (2.19). In this system, the time derivatives for ϕ and k have been omitted and the dynamics is only retained in the equation for the boundary position X.

4.1 Steady-state solutions

To find steady-state solutions

$$X = X_0(y,t), \quad \rho = \rho_0(x,y,t), \quad \phi = \phi_0(y,t), \quad k = k_0(y,t),$$

we consider flat step edges moving with a constant velocity. So, as before, we define $X_0(y,t) = v_0 t$ with $v_0 > 0$ the constant normal velocity of step edges. It follows immediately from (2.1) and (2.2) that the corresponding angle, curvature, and unit normal are given by $\theta_0 = 0$, $\kappa_0 = 0$, and $\mathbf{n}_0 = (1, 0)$, respectively. Since $X_0(y,t)$ is in fact independent of y, we assume that the adatom density is also independent of y, so, $\rho_0 = \rho_0(x,t)$. We also consider constant edge adatom density ϕ_0 and constant kink density k_0. By (2.7), the corresponding left-facing and right-facing kink densities are given by $k_{l0} = k_{r0} = k_0/2$.

Now, by (4.1) – (4.3), (2.11) and (2.12) (or (4.4) and (4.5)), and (2.13) – (2.19), we obtain for both the quasi-steady and steady systems the steady-state solution

$$\begin{aligned}
&X_0(y,t) = v_0 t, \\
&v_0 = 2a^2 FL, \\
&\rho_0(x,t) = -\frac{F}{2D}\left[(x - v_0 t)^2 - L^2\right] + \frac{\beta\phi_0 + FL}{a\alpha} \quad \text{for } v_0 t - L < x < v_0 t + L, \\
&f_{00} = 2f_{+0} = 2f_{-0} = 2FL, \\
&k_0 = \frac{2aFL}{w_0}, \\
&w_0 = a^2(l_{123}\beta\phi_0 + l_{23}FL), \\
&g_0 = a\phi_0(m_{123}\beta\phi_0 + m_{23}FL), \\
&h_0 = \frac{1}{4}a^2 k_0^2(n_{123}\beta\phi_0 + n_{23}FL), \\
&g_0 = h_0,
\end{aligned} \tag{4.6}$$

where for convenience we have used and will use the notation

$$q_{ij} = q_i + q_j \qquad \text{and} \qquad q_{ijk} = q_i + q_j + q_k$$

for $q = l, m$, or n. Note that the last equation determines ϕ_0 which, together with rest of the equations, determines all other quantities.

Define the edge Péclet number $P_e = 2a^3FL/d = 2aFL/\beta$. Set

$$H(\xi, P_e) \;=\; \xi(2m_{123}\xi + m_{23}P_e)(2l_{123}\xi + l_{23}P_e)^2 - P_e^2(2n_{123}\xi + n_{23}P_e), \qquad \xi \in \mathbf{R}.$$

It follows from the above expressions of k_0, w_0, g_0, h_0, and the equation $g_0 = h_0$ that

$$H(a\phi_0, P_e) = \frac{8}{a\beta^3} w_0^2 (g_0 - h_0) = 0.$$

But one easily verifies for each fixed $P_e > 0$ that $H(0, P_e) < 0$, $H(\xi, P_e) \to +\infty$ as $\xi \to \infty$, and $\frac{\partial^2}{\partial \xi^2} H(\xi, P_e) > 0$ for all $\xi \in \mathbf{R}$. Hence, $a\phi_0$ is the unique positive solution of $H(\xi, P_e) = 0$ for the fixed P_e. The steady-state solution (4.6) is therefore unique. Moreover, since $a\phi_0$ depends only on P_e, we can see from (4.6) that ak_0, $w_0/(a\beta)$, ag_0/β, ah_0/β also depend only on P_e. In particular, we have by the k_0 and w_0 equations in (4.6) that

$$ak_0 = \frac{2P_e}{2l_{123}a\phi_0 + l_{23}P_e}.$$

Proposition 4.1 *We have that*

$$a\phi_0 = \left(\frac{n_{123}}{4l_{123}^2 m_{123}}\right)^{1/3} P_e^{2/3} + O(P_e) \quad and \quad ak_0 = \left(\frac{l_{123}n_{123}}{4m_{123}}\right)^{1/3} P_e^{1/3} + O\left(P_e^{2/3}\right) \quad (4.7)$$

as $P_e \to 0$. *We have also that*

$$a\phi_0 = \sigma_0 + \sigma_1 P_e^{-1} + O\left(P_e^{-2}\right) \quad and \quad ak_0 = \frac{2}{l_{23}} - \frac{4l_{123}\sigma_0}{l_{23}^2} P_e^{-1} + O\left(P_e^{-2}\right) \quad (4.8)$$

as $P_e \to \infty$, *where*

$$\sigma_0 = \frac{n_{23}}{l_{23}^2 m_{23}} \quad and \quad \sigma_1 = 2\sigma_0^2 \left(\frac{n_1}{n_{23}} - \frac{m_1}{m_{23}} - \frac{2l_1}{l_{23}} - 2\right).$$

Moreover, if $\sigma_1 < 0$, *then* $a\phi_0$ *is a strictly increasing function of* P_e *in* $(0, \infty)$ *and* $a\phi_0 \to \sigma_0$ *as* $P_e \to \infty$; *if* $\sigma_1 > 0$, *then there exists a* $P_0 > 0$ *such that* $a\phi_0$ *as a function of* P_e *strictly increases in* $(0, P_0)$, $a\phi_0 > \sigma_0$ *in* (P_0, ∞), *and* $a\phi_0 \to \sigma_0$ *as* $P_e \to \infty$.

Proof Both (4.7) and (4.8) can be obtained by a direct calculation based on the fact that $H(a\phi_0, P_e) = 0$.

Set $\xi = a\phi_0$ as a function of P_e. Differentiating both sides of the equation $H(\xi, P_e) = 0$ with respect to P_e, we obtain by a series of calculations that

$$\frac{P_e}{\xi}\xi'(P_e) = \frac{n_{23}P_e^3 - l_{23}^2 m_{23} P_e^3 \xi + 4l_{123}(2l_{23}m_{123} + l_{123}m_{23})P_e\xi^3 + 16l_{123}^2 m_{123}\xi^4}{n_{23}P_e^3 + 2l_{23}(l_{23}m_{123} + 2l_{123}m_{23})P_e^2\xi^2 + 8l_{123}(2l_{23}m_{123} + l_{123}m_{23})P_e\xi^3 + 24l_{123}^2 m_{123}\xi^4}.$$

Consequently, $\xi'(P_e) > 0$ if $\xi \le \sigma_0$. Moreover, if $\sigma_1 < 0$, then $\xi'(P_e) > 0$ for large P_e. Otherwise, if $\sigma_1 > 0$, then $\xi'(P_e) < 0$ for large P_e. These properties, together with (4.8), imply the rest part of the proposition. *Q.E.D.*

We remark that the case when $l_{23} = m_{23} = n_{23} = 0$ is included in our reduced model 1 in Section 5, cf. (5.2). In Figure 4.1, we plot the graphs of $a\phi_0$ and ak_0 as functions of the edge Péclet number P_e with $(l_1, l_2, l_3) = (2, 2, 1)$, $(m_1, m_2, m_3) = (2, 4, 2)$, and $(n_1, n_2, n_3) = (2, 3, 1)$. These are the parameters used in [4]. They satisfy that $\sigma_1 < 0$.

4.2 Linearized systems

Let us formally expand a solution (X, ρ, ϕ, k) around a steady-state solution $(X_0, \rho_0, \phi_0, k_0)$ as follows:

$$X = X_0 + \epsilon X_1, \qquad \rho = \rho_0 + \epsilon\rho_1, \qquad \phi = \phi_0 + \epsilon\phi_1, \qquad k = k_0 + \epsilon k_1,$$

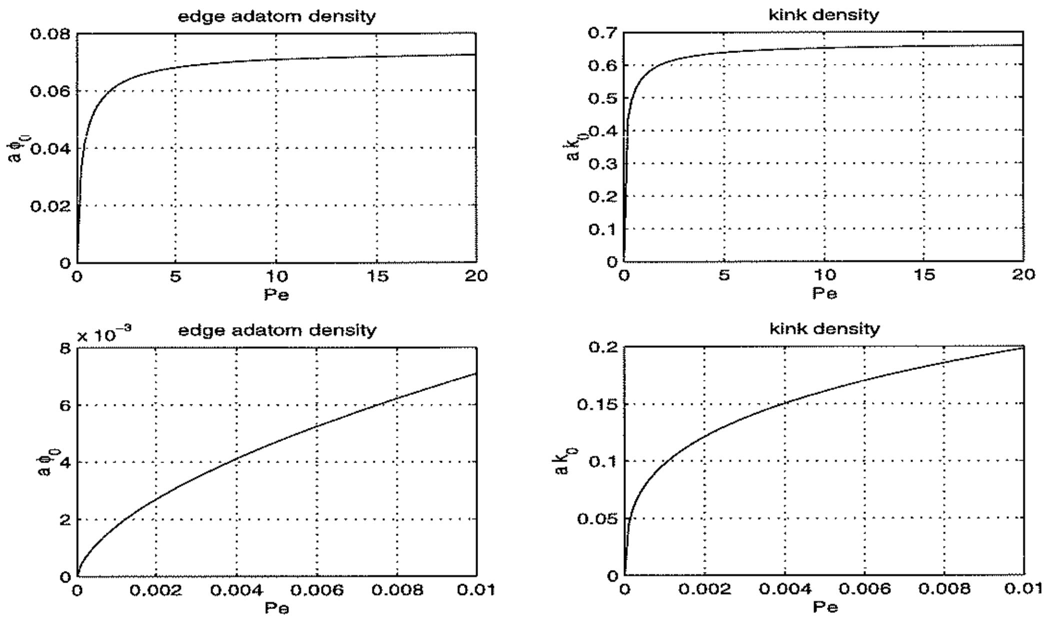

Figure 4.1. The steady-state solutions of the edge adatom density and kink density as functions of the edge Péclet number P_e with $(l_1, l_2, l_3) = (2, 2, 1)$, $(m_1, m_2, m_3) = (2, 4, 2)$, and $(n_1, n_2, n_3) = (2, 3, 1)$.

where ϵ is a small parameter, and $X_1 = X_1(y,t)$, $\rho_1 = \rho_1(x,y,t)$, $\phi_1 = \phi_1(y,t)$, and $k_1 = k_1(y,t)$ are some smooth functions. Expanding also formally

$$\theta = \theta_0 + \epsilon\theta_1, \qquad \kappa = \kappa_0 + \epsilon\kappa_1, \qquad \mathbf{n} = \mathbf{n}_0 + \epsilon\mathbf{n}_1, \qquad v = v_0 + \epsilon v_1,$$

where all θ_1, κ_1, $\mathbf{n}_1$, and v_1 are functions of (y,t), we obtain by using the relations (2.1) and (2.2), and comparing terms of order ϵ that

$$\theta_1 = -\partial_y X_1, \qquad \kappa_1 = \partial_s \theta_1, \qquad \mathbf{n}_1 = (0, \theta_1), \qquad v_1 = \partial_t X_1. \tag{4.9}$$

Notice that from Eq. (2.7),

$$k_l k_r = \frac{1}{4}\left[(k_l + k_r)^2 - (k_l - k_r)^2\right] = \frac{1}{4}\left(k^2 - a^{-2}\tan^2\theta\right) = \frac{1}{4}k^2 + O\left(\epsilon^2\right). \tag{4.10}$$

For convenience, we also expand the related quantities as follows.

$$\begin{aligned} f_+ = f_{+0} + \epsilon f_{+1}, \qquad f_- = f_{-0} + \epsilon f_{-1}, \qquad f_0 = f_{00} + \epsilon f_{01}, \\ w = w_0 + \epsilon w_1, \qquad g = g_0 + \epsilon g_1, \qquad h = h_0 + \epsilon h_1, \end{aligned}$$

where all quantities with subscript 1 are functions of (y,t).

Now, for the quasi-steady system, insert all the above expansions into Eqs. (4.1) – (4.3) and (2.11) – (2.19). Using the steady-state solution (4.6) and the expressions for θ_1,

k_1, $\mathbf{n}_1$, v_1 in (4.9), we then obtain

$$
\begin{aligned}
&\nabla^2 \rho_1 = 0 \qquad \text{for } v_0 t - L < x < v_0 t + L, \\
&D\partial_x \rho_{1+} - FX_1 + f_{+1} = 0 \qquad \text{at } x = v_0 t + L, \\
&D\partial_x \rho_{1-} - FX_1 - f_{-1} = 0 \qquad \text{at } x = v_0 t - L, \\
&\partial_t \phi_1 - d\partial_y^2 \phi_1 = f_{+1} + f_{-1} - f_{01}, \\
&\partial_t k_1 - a^{-1} w_0 \partial_y^2 X_1 = 2(g_1 - h_1),
\end{aligned}
\tag{4.11}
$$

and the constitutive relations

$$
\begin{aligned}
f_{+1} &= \alpha a \rho_{1+} - \beta \phi_1 - a^{-1} FLX_1, \\
f_{-1} &= \alpha a \rho_{1-} - \beta \phi_1 + a^{-1} FLX_1, \\
f_{01} &= -v_0 \phi_0 \partial_y^2 X_1 + a^{-2} \partial_t X_1, \\
w_1 &= aD(l_2 \rho_{1+} + l_3 \rho_{1-}) + l_1 d\phi_1 + (l_3 - l_2) aFLX_1, \\
g_1 &= D\phi_0 (m_2 \rho_{1+} + m_3 \rho_{1-}) + \left(a m_1 \beta \phi_0 + \frac{g_0}{\phi_0} \right) \phi_1 + (m_3 - m_2) FL\phi_0 X_1, \\
h_1 &= \frac{1}{4} a D k_0^2 (n_2 \rho_{1+} + n_3 \rho_{1-}) + \frac{1}{4} n_1 d k_0^2 \phi_1 + \frac{2h_0}{k_0} k_1 + \frac{1}{4} (n_3 - n_2) aFLk_0^2 X_1, \\
\partial_t X_1 &= a w_0 k_1 + a k_0 w_1.
\end{aligned}
\tag{4.12}
$$

The linearized system for the steady system (4.1) – (4.5) and (2.13) – (2.19) is the same except the two time derivative terms $\partial_t \phi_1$ and $\partial_t k_1$ are dropped from the ϕ_1 and k_1 equations in (4.11), respectively.

4.3 Dispersion relations

Let us assume that solutions of the above linear system (4.11) and (4.12) are p-periodic with respect to y for some p. We have from the first equation in (4.11) that ρ_1 has the form

$$
\rho_1 = [\hat{r}_1 \cosh(lx) + \hat{s}_1 \sinh(lx)] \, e^{\omega t + ily}, \tag{4.13}
$$

where $\hat{r}_1$,$\hat{s}_1$ are constants and $pl/2\pi$ is an integer. Set

$$
(\phi_1, k_1, X_1) = \left(\hat{\phi}_1, \hat{k}_1, \hat{X}_1 \right) e^{\omega t + ily}, \tag{4.14}
$$

where $\hat{\phi}_1$, $\hat{k}_1$, and $\hat{X}_1$ are constants. Inserting (4.13) and (4.14) into the two boundary conditions in (4.11), the equations for ϕ_1 and k_1 in (4.11), and the last equation in (4.12), using all the other relations in (4.12), we obtain, after a series of calculations, that

$$
\begin{aligned}
&\alpha \left[a^2 l \cosh(lL) + a \sinh(lL) \right] \hat{s}_1 - F \left(1 + a^{-1} L \right) \hat{X}_1 = 0, \\
&\alpha \left[a^2 l \sinh(lL) + a \cosh(lL) \right] \hat{r}_1 - \beta \hat{\phi}_1 = 0,
\end{aligned}
$$

$$2\alpha a\cosh(lL)\hat{r}_1 - \left(2\beta + dl^2 + \omega\right)\hat{\phi}_1 + \left(-v_0\phi_0 l^2 - a^{-2}\omega\right)\hat{X}_1 = 0, \tag{4.15}$$
$$\alpha G_r\cosh(lL)\hat{r}_1 + \alpha G_s\sinh(lL)\hat{s}_1 + G_\phi\hat{\phi}_1 + (G_k - \omega)\hat{k}_1 + \left(G_X - a^{-1}w_0 l^2\right)\hat{X}_1 = 0,$$
$$\alpha V_r\cosh(lL)\hat{r}_1 + \alpha V_s\sinh(lL)\hat{s}_1 + V_\phi\hat{\phi}_1 + V_k\hat{k}_1 + (V_X - \omega)\hat{X}_1 = 0,$$

where

$$\begin{aligned}
G_r &= 2m_{23}a^2\phi_0 - \frac{1}{2}n_{23}a^3k_0^2,\\
G_s &= 2(m_2 - m_3)a^2\phi_0 - \frac{1}{2}(n_2 - n_3)a^3k_0^2,\\
G_\phi &= 2m_1 a\beta\phi_0 + \frac{2g_0}{\phi_0} - \frac{1}{2}n_1 dk_0^2,\\
G_k &= -\frac{4h_0}{k_0},\\
G_X &= 2(m_3 - m_2)FL\phi_0 - \frac{1}{2}(n_3 - n_2)ak_0^2FL,
\end{aligned} \tag{4.16}$$

and

$$\begin{aligned}
V_r &= l_{23}a^4k_0,\\
V_s &= (l_2 - l_3)a^4k_0,\\
V_\phi &= l_1 adk_0,\\
V_k &= aw_0,\\
V_X &= (l_3 - l_2)a^2k_0FL.
\end{aligned} \tag{4.17}$$

There is a nonzero solution $(X_1, \rho_1, \phi_1, k_1)$ of the form (4.13), (4.14) if and only if the determinant of the coefficient matrix of the above linear system (4.15) for $(\hat{r}_1, \hat{s}_1, \hat{\phi}_1, \hat{k}_1, \hat{X}_1)$ vanishes. Notice that this determinant is zero if $l = 0$. Assume now $l \neq 0$. Factoring $\alpha\cosh(lL)$ and $\alpha\sinh(lL)$ from the first and second columns of the determinant, respectively, we see that the condition that the determinant is zero becomes

$$\begin{vmatrix}
0 & a^2 l\coth(lL) + a & 0 & 0 & -F\left(1 + a^{-1}L\right)\\
a^2 l\tanh(lL) + a & 0 & -\beta & 0 & 0\\
2a & 0 & -\left(2\beta + dl^2 + \omega\right) & 0 & -v_0\phi_0 l^2 - a^{-2}\omega\\
G_r & G_s & G_\phi & G_k - \omega & G_X - a^{-1}w_0 l^2\\
V_r & V_s & V_\phi & V_k & V_X - \omega
\end{vmatrix} = 0. \tag{4.18}$$

This determines the dispersion relation $\omega = \omega(l)$ with $l \neq 0$ for the quasi-steady system.

For the steady system, we obtain similarly that

$$\begin{vmatrix}
0 & a^2 l\coth(lL) + a & 0 & 0 & -F\left(1 + a^{-1}L\right)\\
a^2 l\tanh(lL) + a & 0 & -\beta & 0 & 0\\
2a & 0 & -\left(2\beta + dl^2\right) & 0 & -v_0\phi_0 l^2 - a^{-2}\omega\\
G_r & G_s & G_\phi & G_k & G_X - a^{-1}w_0 l^2\\
V_r & V_s & V_\phi & V_k & V_X - \omega
\end{vmatrix} = 0, \tag{4.19}$$

which determines the dispersion relation $\omega = \omega(l)$ for $l \neq 0$ in the steady case.

A simple manipulation of the above determinants using the fact that all $v_0/(a\beta)$, $w_0/(a\beta)$, $a\phi_0$, and ak_0 depend only on the edge Péclet number P_e shows that these dispersion relations are of the form $\omega(l) = \beta S\left(L/a, P_e, al\right)$, where S is a function of three variables. In particular, the dispersion relation is independent of the adatom hopping rate α for both the steady and quasi-steady systems.

4.4 Asymptotic analysis

Denote for each $l \geq 0$ by $\omega = \omega(l)$ the root of the linear equation (4.19) and by $\omega_1 = \omega_1(l), \omega_2 = \omega_2(l)$, and $\omega_3 = \omega_3(l)$ the three roots of the cubic equation (4.18). Assume that $\omega_1(l)$ is always real, and $\omega_1(0) = 0$ since $w = 0$ is a solution of (4.18) for $l = 0$.

Proposition 4.2 *For the steady system, we have*

$$\omega(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right) \qquad \text{as } l \to 0, \tag{4.20}$$

$$\omega(l) = -\frac{v_0 w_0}{4ah_0} l^2 + O\left(1\right) \qquad \text{as } l \to \infty. \tag{4.21}$$

For the quasi-steady system, we have

$$\omega_1(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right) \qquad \text{as } l \to 0, \tag{4.22}$$

and

$$\begin{aligned} \omega_1(l) &= -dl^2 + O(l), \\ \omega_2(l) &= R_0 + iw_0 l + O\left(l^{-1}\right), \\ \omega_3(l) &= R_0 - iw_0 l + O\left(l^{-1}\right), \end{aligned} \tag{4.23}$$

as $l \to \infty$, where $i = \sqrt{-1}$ and

$$R_0 = \frac{\beta a k_0}{4}\left[(l_3 - l_2 - n_{23})P_e - 2n_{123} a\phi_0 - 2l_1 P_e a\phi_0\right]. \tag{4.24}$$

Moreover, $R_0 < 0$ for small edge Péclet number P_e. A sufficient condition for $R_0 < 0$ for all $P_e > 0$ is that

$$l_3 - l_2 - n_{23} \leq 0, \tag{4.25}$$

and a necessary condition for $R_0 < 0$ for all $P_e > 0$ is that

$$(l_3 - l_2 - n_{23}) l_{23}^2 m_{23} - 2l_1 n_{23} \leq 0. \tag{4.26}$$

Proof Consider first the steady system. By (4.19) we have $\omega(l) = A(l)/B(l)$, where

$$A(l) = \begin{vmatrix} 0 & a^2 l \coth(lL) + a & 0 & 0 & -F\left(1 + a^{-1}L\right) \\ a^2 l \tanh(lL) + a & 0 & -\beta & 0 & 0 \\ 2a & 0 & -\left(2\beta + dl^2\right) & 0 & -v_0\phi_0 l^2 \\ G_r & G_s & G_\phi & G_k & G_X - a^{-1}w_0 l^2 \\ V_r & V_s & V_\phi & V_k & V_X \end{vmatrix},$$

$$B(l) = \begin{vmatrix} 0 & a^2 l \coth(lL) + a & 0 & 0 & 0 \\ a^2 l \tanh(lL) + a & 0 & -\beta & 0 & 0 \\ 2a & 0 & -\left(2\beta + dl^2\right) & 0 & a^{-2} \\ G_r & G_s & G_\phi & G_k & 0 \\ V_r & V_s & V_\phi & V_k & 1 \end{vmatrix}.$$

By expanding $A(l)$ and $B(l)$ along the first row and the last column, respectively, we obtain that

$$A(l) = a^2 v_0 \phi_0 q_0 l^2 + O(l^4) \quad \text{and} \quad B(l) = -q_0 + O(l^2) \quad \text{as } l \to 0,$$

where

$$q_0 = \begin{vmatrix} a & -\beta & 0 \\ G_r & G_\phi & G_k \\ V_r & V_\phi & V_k \end{vmatrix} = 4 l_{123} a^4 \beta h_0 + 2 m_{123} a^3 \beta \phi_0 w_0 + \frac{1}{2\phi_0} n_{23} a^4 k_0^2 w_0 F L > 0,$$

and that

$$A(l) = a^4 \beta w_0^2 l^6 + O(l^4) \quad \text{and} \quad B(l) = a^4 \beta G_k l^4 + O(l^2) \quad \text{as } l \to \infty.$$

These imply (4.20) and (4.21) immediately.

Consider now the quasi-steady system. Notice first that $\omega_1(l) \to \omega_1(0) = 0$ as $l \to 0$. By a series of calculations, we obtain from (4.18) that

$$q_0\left(\omega_1(l) + a^2 v_0 \phi_0 l^2\right) + O\left(l^4\right) + O\left(l^2 \omega_1(l)\right) + O\left(\omega_1(l)^2\right) = 0 \quad \text{as } l \to 0,$$

implying (4.22).

Observe from (4.18) that $|\omega(l)| \to \infty$ as $l \to \infty$. A simple manipulation of the determinant (4.18) leads to

$$\begin{vmatrix} -\left(2\beta + dl^2 + \omega\right) & 0 & -v_0\phi_0 l^2 - a^{-2}\omega \\ G_\phi & G_k - \omega & G_X - a^{-1} w_0 l^2 \\ V_\phi & V_k & V_X - \omega \end{vmatrix} + O(l|\omega|) + O\left(|\omega|^2/l\right) = 0,$$

for large l. Consequently,

$$\omega^3 + dl^2\omega^2 + \left(2\beta + a^{-2}V_\phi - G_k - V_X\right)\omega^2 + \left(w_0^2 - dG_k - dV_X + V_\phi v_0 \phi_0\right) l^2 \omega$$
$$+ d w_0^2 l^4 + O(l|\omega|) + O\left(|\omega|^2/l\right) + O\left(l^2\right) = 0 \qquad \text{as } l \to \infty. \tag{4.27}$$

It then follows immediately that there exist constants $c_1 > 0$ and $c_2 > 0$ such that

$$c_1 l \le |\omega(l)| \le c_2 l^2 \qquad \text{for large } l.$$

If $|\omega(l)|/l^2$ is bounded below by a positive constant for large l, then (4.27) implies that

$$\omega(l) = -dl^2 + O(l) \qquad \text{as } l \to \infty. \tag{4.28}$$

If on the other hand, up to a subsequence of $\{l\}$, $\omega(l)/l^2 \to 0$ as $l \to \infty$, then we must have that $\omega(l) = O(l)$, for otherwise, we would have a contradiction from (4.27). Therefore, the highest order terms in (4.27) are those of $l^2\omega^2$ and l^4. Consequently, we have

$$\omega(l) = R(l) + i\sigma w_0 l \qquad \text{as } \to l, \tag{4.29}$$

where $R(l)$ is a bounded function of l and $\sigma = 1$ or -1. If we plug the above expression back into (4.27), we then have

$$R(l) = R_0 + O\left(l^{-1}\right) \qquad \text{as } l \to \infty, \tag{4.30}$$

where R_0 is defined by (4.24). Now, (4.23) follows from (4.28) – (4.30).

Finally, the fact that $R_0 < 0$ for small edge Péclet number P_e follows from (4.7). The condition (4.25) is obviously sufficient for $R_0 < 0$ for all P_e. The necessary condition (4.26) follows from the asymptotic expansion for $a\phi_0$ in (4.8). *Q.E.D.*

5 Model reduction

We present three reduced attachment-detachment models and study their linear stability. Skipping details of the analysis which are similar to those for the original model, we summarize the stability result in Section 5.4.

5.1 Reduced model 1

This model is the same as that of the original attachment-detachment model except that the expressions of w, g, and h in (2.16) – (2.18) are simplified as

$$w = l_1 d\phi, \qquad g = m_1 a\beta\phi^2, \qquad h = n_1 d\phi k_r k_l, \tag{5.1}$$

which result from the assumption that $l_2 = l_3 = m_2 = m_3 = n_2 = n_3 = 0$.

The steady-state solutions of $X_0, v_0, \rho_0, f_{+0}, f_{-0}$, and f_0 are the same as given in (4.6), but those of ϕ_0, k_0, w_0, g_0, and h_0 are given by

$$a\phi_0 = \frac{n_1}{4m_1}(ak_0)^2, \qquad ak_0 = \left(\frac{4m_1}{l_1 n_1} P_e\right)^{1/3}, \tag{5.2}$$

$$\frac{w_0}{a\beta} = l_1 a\phi_0, \qquad \frac{ag_0}{\beta} = m_1 (a\phi_0)^2, \qquad \frac{ah_0}{\beta} = \frac{1}{4} n_1 (a\phi_0)(ak_0)^2, \tag{5.3}$$

where $P_e = 2aFL/\beta$ is the edge Péclet number. Notice that $a\phi_0, ak_0, w_0/(a\beta), ag_0/\beta$, and ah_0/β are still functions of P_e only. But they are no longer bounded.

The linearized system for the quasi-steady system is the same as that given in (4.11) and (4.12) except the equations for w_1, g_1, and h_1 are simplified as

$$w_1 = l_1 d\phi_1, \qquad g_1 = 2m_1 a\beta\phi_0\phi_1, \qquad h_1 = \frac{1}{4}n_1 dk_0^2\phi_1 + \frac{1}{2}n_1 d\phi_0 k_0 k_1. \tag{5.4}$$

The linearized system for the steady system can be obtained from (4.11) and (4.12) by dropping the two time derivative terms $\partial_t\phi_1$ and $\partial_t k_1$ in the ϕ_1 and k_1 equations in (4.11), respectively, and replacing the expressions of w_1, g_1, and h_1 there by those in (5.4).

Assume that the solutions to the linearized systems are periodic. Then, ρ_1 is given by (4.13) and (ϕ_1, k_1, X_1) has the form (4.14). Consequently, by a series of calculations similar to those in Section 4, we obtain the following dispersion relations

$$\begin{vmatrix} a^2 l\tanh(lL) + a & -\beta & 0 & 0 \\ 2a & -(2\beta + dl^2 + \omega) & 0 & -v_0\phi_0 l^2 - a^{-2}\omega \\ 0 & \frac{1}{2}n_1 dk_0^2 & -(n_1 d\phi_0 k_0 + \omega) & -a^{-1}w_0 l^2 \\ 0 & l_1 adk_0 & aw_0 & -\omega \end{vmatrix} = 0 \tag{5.5}$$

and

$$\begin{vmatrix} a^2 l\tanh(lL) + a & -\beta & 0 & 0 \\ 2a & -(2\beta + dl^2) & 0 & -v_0\phi_0 l^2 - a^{-2}\omega \\ 0 & \frac{1}{2}n_1 dk_0^2 & -n_1 d\phi_0 k_0 & -a^{-1}w_0 l^2 \\ 0 & l_1 adk_0 & aw_0 & -\omega \end{vmatrix} = 0 \tag{5.6}$$

for the quasi-steady system and steady system, respectively. They are again of the form $\omega(l) = \beta S(L/a, P_e, al)$ with S a function of three variables, and are independent of the adatom hopping rate α. From (5.6), (5.2), (5.3), and (4.6), we obtain for the steady system that

$$\omega(l) = -\frac{\beta\left[(al)\tanh(lL) + 1\right]\left[\frac{3n_1}{2l_1}P_e^3 + \left(\frac{w_0}{a\beta}\right)^2 (al)^2\right](al)^2 + 2\left(\frac{w_0}{a\beta}\right)^2 (al)^3\tanh(lL)}{\left[(al)\tanh(lL) + 1\right]\left[\frac{3}{2}n_1 P_e(ak_0) + \frac{n_1}{l_1}P_e(al)^2\right] + \frac{2n_1}{l_1}P_e(al)\tanh(lL)}. \tag{5.7}$$

5.2 Reduced model 2

For the simplicity of numerical simulation, we now propose the second reduced model by further dropping all the derivative terms in the ϕ and k equations in the first reduced model. So, this one is the same as the first reduced model except that the ϕ and k equations (2.11) and (2.12) are replaced by

$$f_+ + f_- = f_0 \qquad \text{and} \qquad g = h,$$

respectively.

The steady-state solution of this system is the same as that of the steady system of reduced model 1. The corresponding linearized system consists of equations (4.11) and (4.12) with the ϕ_1 and k_1 equations replaced by

$$f_{+1} + f_{-1} = f_{01} \qquad \text{and} \qquad g_1 = h_1,$$

and the w_1, g_1, and h_1 equations replaced by (5.4), respectively. As before, we assume that the solutions to the linearized systems are periodic. Then, ρ_1 is given by (4.13) and (ϕ_1, k_1, X_1) has the form (4.14). The dispersion relation is given by (cf. (5.5))

$$\begin{vmatrix} a^2 l \tanh(lL) + a & -\beta & 0 & 0 \\ 2a & -2\beta & 0 & -v_0\phi_0 l^2 - a^{-2}\omega \\ 0 & \frac{1}{2}n_1 d k_0^2 & -n_1 d\phi_0 k_0 & 0 \\ 0 & l_1 a d k_0 & a w_0 & -\omega \end{vmatrix} = 0,$$

which leads to

$$\omega(l) = -\frac{3l_1 a^2 v_0 \phi_0 k_0 \left[al\tanh(lL) + 1\right] l^2}{3l_1 k_0 \left[al\tanh(lL) + 1\right] + 4l\tanh(lL)}. \tag{5.8}$$

This is also of the form $\omega(l) = \beta S\left(L/a, P_e, al\right)$ with S a function of three variables, and is independent of the adatom hopping rate α.

5.3 Reduced model 3

Motivated by the observation that the dispersion relation is independent on the terrace hopping rate α for the quasi-steady and steady systems, we now develop the third reduced attachment-detachment model that does not involve the adatom density to study the stabilizing role of the edge diffusion and kink convection. By assuming that the adatoms diffuse infinitely fast and attach uniformly to step edges, we have that the adatom density on steps is $\rho = 0$ and that the total flux to a step edge is $f_+ + f_- = 2FL$. By assuming also that there is no detachment of atoms from an edge or a kink to a step, we get from the original attachment-detachment model that

$$\begin{aligned} &\partial_t\phi - d\partial_s^2\phi = 2FL + f_0, \\ &\partial_t k + \partial_s(w(k_r - k_l)) = 2(g - h), \\ &v = awk\cos\theta, \end{aligned}$$

where f_0 is given in (2.15), k_r and k_l satisfy (2.7), and w, g, and h are given in (5.1). Equivalently (cf. (4.10)),

$$\begin{aligned} &\partial_t\phi - d\partial_s^2\phi = 2FL + v\left(\phi\partial_s\theta - a^{-2}\right), \\ &\partial_t k - l_1 a\beta\partial_s(\phi\partial_y X) = 2m_1 a\beta\phi^2 - \frac{1}{2}n_1 d\phi k^2 + \frac{1}{2}n_1\beta\phi(\partial_y X)^2, \\ &v = l_1 a d\phi k\cos\theta. \end{aligned} \tag{5.9}$$

These are the governing equations of this reduced model for edge adatom diffusion and kink convection.

For this model, the steady-state solutions X_0, v_0, ϕ_0, and k_0 are the same as those in reduced model 1. The linearized system around the steady-state solution is given by

$$\begin{aligned}
&\partial_t\phi_1 - d\partial_y^2\phi_1 + a^{-2}\partial_t X_1 - v_0\phi_0\partial_y^2 X_1 = 0,\\
&\frac{1}{2}n_1 d k_0^2\phi_1 - \partial_t k_1 - n_1 d\phi_0 k_0 k_1 + l_1 a\beta\phi_0\partial_y^2 X_1 = 0,\\
&l_1 a d k_0\phi_1 + l_1 a d\phi_0 k_1 - \partial_t X_1 = 0.
\end{aligned} \tag{5.10}$$

Setting as before

$$(\phi_1, k_1, X_1) = \left(\hat{\phi}_1, \hat{k}_1, \hat{X}_1\right) e^{\omega t + ily},$$

we then obtain the following dispersion relation

$$\begin{vmatrix}
\omega + dl^2 & 0 & a^{-2}\omega + v_0\phi_0 l^2 \\
\frac{1}{2}n_1 d k_0^2 & -\omega - n_1 d\phi_0 k_0 & -l_1 a\beta\phi_0 l^2 \\
l_1 a d k_0 & l_1 a d\phi_0 & -\omega
\end{vmatrix} = 0,$$

which is equivalent to

$$\left(\frac{\omega}{\beta}\right)^3 + \left[(al)^2 + \frac{n_1 P_e}{l_1} + l_1(ak_0)\right]\left(\frac{\omega}{\beta}\right)^2 + \left\{\left[\frac{n_1}{l_1}P_e + P_e^2 + l_1^2(a\phi_0)^2\right](al)^2 + \frac{3}{2}n_1 P_e(ak_0)\right\}\frac{\omega}{\beta} + \left[\frac{3n_1}{2l_1}P_e^3(al)^2 + l_1^2(a\phi_0)^2(al)^4\right] = 0. \tag{5.11}$$

If we drop the terms $\partial_t\phi$ and $\partial_t k$ in (5.9), we obtain the corresponding steady system. It has the same steady-state solution. And the corresponding linearized system can be obtained by dropping the two terms $\partial_t\phi_1$ and $\partial_t k_1$ in (5.10). The dispersion relation in this case can be obtained explicitly as

$$\omega(l) = -\frac{l_1\beta(a\phi_0)(al)^2\left[2l_1(al)^2 + 3n_1 P_e(ak_0)^2\right]}{n_1(ak_0)\left[2(al)^2 + 3l_1(ak_0)\right]}. \tag{5.12}$$

Notice that the dispersion relation for both the steady and unsteady systems of this model is of the form $\omega = \beta T(P_e, al)$ with T a function of two variables.

5.4 Stability results and comparison

As for the original attachment-detachment model, we denote by $\omega = \omega(l)$ the frequency function determined by (5.7), (5.8), and (5.12) for the steady-systems of the reduced models, respectively. We also denote for each $l \geq 0$ by $\omega_1 = \omega_1(l), \omega_2 = \omega_2(l)$, and $\omega_3 = \omega_3(l)$ the three roots of the cubic equations (5.5) and (5.11) for the quasi-steady system of the reduced model 1 and 3, respectively. We can assume as before that $\omega_1(l)$ is always real and $\omega_1(0) = 0$. We summarize our stability results for the reduced models as well as the original attachment-detachment model in Table 5.1.

Model	Steady System	Quasi-steady System
original	$\omega(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right)$ as $l \to 0$ $\omega(l) = -\frac{v_0 w_0}{4ah_0} l^2 + O\left(1\right)$ as $l \to \infty$	$\omega_1(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right)$ as $l \to 0$ $\omega_1(l) = -dl^2 + O(1)$ as $l \to \infty$ $\omega_2(l) = R_0 + i w_0 l + O\left(l^{-1}\right)$ as $l \to \infty$ $\omega_3(l) = R_0 - i w_0 l + O\left(l^{-1}\right)$ as $l \to \infty$
1	$\omega(l) < 0$ for all $l > 0$ $\omega_1(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right)$ as $l \to 0$ $\omega(l) = -\frac{v_0 w_0}{4ah_0} l^2 + O(l)$ as $l \to \infty$	$\omega_1(0) = 0$, $\mathrm{Re}\left(\omega_j(0)\right) < 0$ $(j = 2, 3)$ $\omega_1(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right)$ as $l \to 0$ $\omega_1(l) = -dl^2 + O(1)$ as $l \to \infty$ $\omega_2(l) = -\frac{1}{2}\beta P_e(P_e + \frac{n_1}{l_1})$ $+ i w_0 l + O\left(l^{-1}\right)$ as $l \to \infty$ $\omega_3(l) = -\frac{1}{2}\beta P_e(P_e + \frac{n_1}{l_1})$ $- i w_0 l + O\left(l^{-1}\right)$ as $l \to \infty$
2	$\omega(l) < 0$ for all $l > 0$ $\omega(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right)$ as $l \to 0$ $\omega(l) = -\frac{3dP_e^2}{3l_1 ak_0 + 4} l^2 + O(l)$ as $l \to \infty$	
3	$\omega(l) < 0$ for all $l > 0$ $\omega(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right)$ as $l \to 0$ $\omega(l) = -\frac{v_0 w_0}{4ah_0} l^2 + O(1)$ as $l \to \infty$	$\omega_1(0) = 0$, $\mathrm{Re}\left(\omega_j(0)\right) < 0$ $(j = 2, 3)$ $\omega_1(l) = -a^2 v_0 \phi_0 l^2 + O\left(l^4\right)$ as $l \to 0$ $\omega_1(l) = -dl^2 + O(1)$ as $l \to \infty$ $\omega_2(l) = -\frac{1}{2}\beta P_e(P_e + \frac{n_1}{l_1})$ $+ i w_0 l + O\left(l^{-1}\right)$ as $l \to \infty$ $\omega_3(l) = -\frac{1}{2}\beta P_e(P_e + \frac{n_1}{l_1})$ $- i w_0 l + O\left(l^{-1}\right)$ as $l \to \infty$

Table 5.1. A summary of the stability results.

In Figure 5.1, we plot the graphs of frequency vs. wave number for various models with a same set of parameters: (a) the steady systems for the original, reduced model 1, and reduced model 3; (b) the quasi-steady for the original and reduced model 1, and the unsteady system of the reduced model 3; (c) the quasi-steady system for the reduced model 1 and the unsteady system of the reduced model 3; and (d) the steady system for the original and reduced model 2. In (b) and (c), ω_m is the maximal value of the real part of $\omega_i(l), i = 1, 2, 3$.

We can now draw several conclusions from our analysis.

- All the leading terms in the asymptotic expansions of $\omega = \omega(l)$ and $\omega_j(l)$ $(j = 1, 2, 3)$ for small and large wave numbers are of the form $-\beta u(P_e)(al)^\sigma$ with $u(\cdot)$ a single variable function and $\sigma \geq 0$ an integer. Thus, the asymptotic stability depends only on the edge Péclet number P_e and edge adatom hopping rate β.

- For all the steady, quasi-steady, and unsteady systems of all the models, we have the same asymptotic expansion of the frequency for small wave numbers. The coefficient of the leading order term $-a^2 v_0 \phi_0$ comes from the curvature term in the expression of f_0 (cf. (2.15)). Hence, for small wave numbers, the stability is determined by the

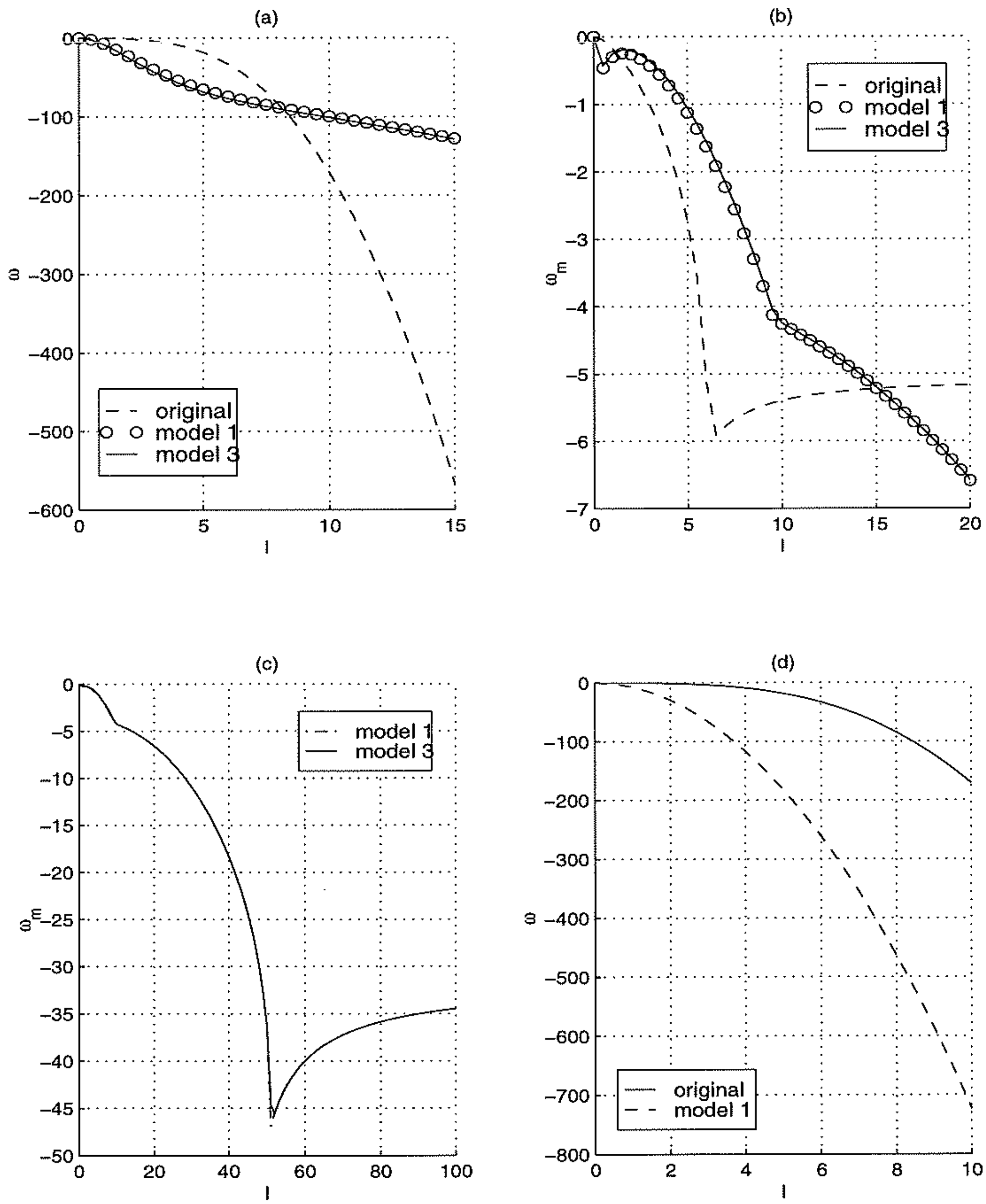

Figure 5.1. Plots of frequencies vs. the wave number for various models. Parameters: $a = 1, \beta = 0.1, F = 0.025, L = 50, (l_1, l_2, l_3) = (2, 2, 1), (m_1, m_2, m_3) = (2, 4, 2), (n_1, n_2, n_3) = (2, 3, 1)$.

geometric effect. However, for large wave numbers, the stability is dominated by the edge diffusion and kink convection.

- For parameters in practice, the original attachment-detachment model is mathematically well-posed. Our numerical calculations with typical parameters further show that the frequency function $\omega(l)$ is always negative for any $l > 0$ for the steady system (cf. Figure 5.1 (a, d)), and that the real parts of $\omega_1(l), \omega_2(l)$, and $\omega_3(l)$ for any $l > 0$ are always negative as well for the quasi-steady system (cf. Figure 5.1 (b)). Therefore, for parameters in application, particularly those used in [4], both the steady and quasi-steady systems of the original model are stable for all the wave numbers.

- All the reduced attachment-detachment models are mathematically well-posed. In fact, their steady systems are stable for all wave numbers. Our numerical calculations show that, for parameters in the range of application, their quasi-steady system are also stable for any wave numbers, cf. Figure 5.1.

- The reduced model 2 is always stable. Recall that this model is obtained from the reduced model 1 by dropping all the derivative terms in the edge diffusion and kink convection equations. Thus, the presence of the edge adatom density and kink density in an attachment-detachment model seems to be more essential than their evolution in stabilizing the system. Meanwhile, the reduced model 2 can provide possibly a good model for numerical simulation, since it needs only to solve the differential equation of the adatom density and the *algebraic equations* of the edge adatom density and kink density.

- The asymptotic expansions of the dispersion relation for the reduced model 1 and 3 are exactly the same. In particular, for the steady system, the coefficients of the l^2 term in these expansions for large wave number l are the same in form as that for the original model. (Note that h_0 has a different expression for the original model.) Consequently, the reduced model 3 is an accurate approximation model for studying the edge diffusion and kink convection.

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