Physica D 241 (2012) 1179–1189

Contents lists available at SciVerse ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

Homogenization of composite vicinal surfaces: Evolution laws in 1 + 1 dimensions

Dionisios Margetis [a,b,c,*], Kanna Nakamura [a]

[a] *Department of Mathematics, University of Maryland, College Park, MD 20742, United States*
[b] *Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742, United States*
[c] *Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, MD 20742, United States*

ARTICLE INFO

Article history:
Received 6 August 2011
Received in revised form
8 February 2012
Accepted 26 March 2012
Available online 1 April 2012
Communicated by A. Mikhailov

Keywords:
Crystal surface
Burton–Cabrera–Frank (BCF) model
Line defects
Diffusion
Macroscopic limit
Multiscale expansion

ABSTRACT

We apply classical homogenization to derive macroscopic relaxation laws for crystal surfaces with *distinct inhomogeneities* at the microscale. The proposed method relies on a formal multiscale expansion in one spatial coordinate. This approach transcends the coarse graining applied previously via Taylor expansions. Our work offers an extension of the static homogenization formulated in a brief report [D. Margetis, Homogenization of reconstructed crystal surfaces: Fick's law of diffusion, Phys. Rev. E 79 (2009) 052601] to account for surface evolution. The starting point is the Burton–Cabrera–Frank (BCF) model for the motion of line defects (steps) separating nanoscale terraces. We enrich this model with sequences of distinct material parameters, i.e., disparate diffusivities of adsorbed atoms (adatoms) across terraces, kinetic sticking rates at step edges, and step energy parameters for elastic-dipole interactions. Multiscale expansions for the adatom concentration and flux are used, with a slow diffusive time scale consistent with the quasi-steady regime for terrace diffusion. The ensuing macroscopic, nonlinear evolution laws incorporate averages of the microscale parameters.

1. Introduction

Crystal surface structures are critical ingredients of thin film epitaxy as well as surface chemistry and catalysis. Aspects of surface evolution remain an area of active interest [1–3]. A crucial issue is to elucidate how the microscale dynamics of constituent atomic defects influence the surface morphological evolution at large scales. This concern broadly motivates the present paper.

Vicinal crystal surfaces are characterized by nanoscale flat regions (terraces) oriented in the high-symmetry direction and separated by line defects (steps) which are typically one atomic layer high. The steps considered here are monotonic (of the same 'sign'). Their number is fixed by the miscut angle set in laboratory experiments [2].

A standard approach to deriving macroscopic limits of stepped surfaces essentially relies on Taylor expansions for the step positions and step density; see, e.g., [4–9]. This coarse graining is appropriate when material parameters remain unchanged across terraces. However, this approach is in principle inadequate if the surface has strong inhomogeneities, namely, distinct diffusivities and kinetic rates across terraces at the nanoscale. We herein call such a stepped surface 'composite'.

In this paper, we address the question: What is the macroscale description of surface relaxation consistent with the microstructure inhomogeneities of a composite stepped surface? To provide an answer, we invoke singular perturbations, i.e., classical homogenization and multiscale expansions, in one spatial coordinate. This approach is deemed more general than the previously applied coarse graining. Our main results comprise evolution laws that contain microscale averages of material parameters.

It is tempting to claim that homogenization is not needed since the requisite averaging may stem from an electric circuit analog for the stepped surface [6,10]. In this view, for instance, sequences of terrace diffusivities correspond to in-series electric conductances per unit length; hence, the average diffusivity would be the appropriate, effective circuit parameter. We believe that this view is incomplete for at least two reasons. First, it is static, leaving out the issue of time scales and evolution. Second, in this picture effective circuit parameters are determined at the (microscale) level of a few steps and terraces. This way of determining effective parameters is conceptually different from the averaging required by homogenization in the macroscopic limit.

The present work forms an extension of a recent, brief report on Fick's law for surface diffusion [11]. Here, more details on the

---

[*] Corresponding author at: Department of Mathematics, University of Maryland, College Park, MD 20742, United States. Tel.: +1 301 405 5455; fax: +1 301 314 0827.

E-mail addresses: dio@math.umd.edu (D. Margetis), nakamura@math.umd.edu (K. Nakamura).

0167-2789/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.physd.2012.03.007

derivation of Fick's law are provided, the roles of time scales and the mesoscale are quantified and discussed extensively, and the continuum laws comprise more variables, e.g., the step chemical potential (a thermodynamic force).

Our analysis is formal, leaving open questions. The main focus is the *consistency* of macroscopic laws with a microscale model of a composite surface. Accordingly, the continuum limit is *assumed* to exist. Our derivation of Fick's law relies on arguments in terms of the classical solution for a microscale diffusion equation. Strictly speaking, our asymptotic (multiscale) expansion approach is mathematically inadequate since the related coefficients of the diffusion equation do not satisfy certain regularity assumptions. Here, we do not address this issue, circumventing the use of more elaborate techniques [12,13]. Instead, we aim to give some intuition and guidance for further, more mathematically rigorous analysis by exemplifying physical assumptions and the core elements of the homogenization procedure.

We restrict attention to one spatial coordinate; and do not study composite stepped surfaces in full $2+1$ dimensions. We believe that the extension of continuum laws to $2+1$ dimensions would require a modified homogenization approach. This case is discussed in Section 4.

We assume that the reader is familiar with the basic concepts of epitaxial relaxation. For reviews on related topics, see, e.g., [1,2,14,3,15].

1.1. Physical motivation

There are at least two categories of applications that physically motivate our study. First, semiconductor surfaces may naturally exhibit structural phases that depend on the temperature and crystal misorientation angle. This "surface reconstruction" amounts to material parameters that can vary appreciably across adjacent terraces and has received considerable attention. In particular, the Si(001) system manifests a reconstruction in which dimer rows (chains of bonded atoms) alternate from perpendicular to parallel to step edges across terraces [16–19].

Another category of phenomena involves surface compounds created by small amounts of solutes added on a crystal. Such additions can cause dramatic morphological changes, affecting the crystal shape and stability [20–24]. This observation implies that artificial, composite surfaces may have interesting, unconventional properties, and need to be explored systematically.

A feature common to both of the above cases is the existence of microstructure inhomogeneities. However, it is reasonable to expect that the surface appears homogeneous at a large enough length scale.

1.2. Averaging and mesoscale

Our homogenization approach is adopted from the basic theory of composites, e.g., [25,26]. The central theme is to identify separate scales from the physical setting and governing equations for steps, and then average out microscopic details in order to pass to the full continuum limit. The averaging procedure is intimately connected to the structure of the governing laws at the microscale. By requiring that classical solutions, e.g., the mass concentration and flux, of step flow remain bounded in the limit that the number of steps is large, one can obtain a "solvability condition" giving rise to an effective macroscopic description.

In this framework, the notion of the *mesoscale* arises naturally [25]. Intuitively, one may think of the mesoscale as a surface region small enough to capture the underlying inhomogeneities yet sufficiently large to allow for reliable averaging. The variation of material parameters and variables (e.g., step velocity) across steps and terraces is evident at the mesoscale; but the corresponding averages of interest vary slowly across such mesoscale regions so that the full continuum limit makes sense.

The above idea permeates the study of diffusion in layered media [27]. The homogenization scheme in [27] is static from the outset; and includes the layer boundaries through the values of a fast, continuous spatial variable. The mass (adatom) concentration and flux are assumed to be continuous across these boundaries [27]. In contrast, our setting encompasses relaxation *dynamics*. The step edges (terrace boundaries) are moving; hence, the step velocity law and step interactions play a role. Furthermore, densities and fluxes are in principle discontinuous across step edges because of the assumed attachment–detachment kinetics at steps. The microscale Fick's law for diffusion is complemented with the step chemical potential.

1.3. Kinetic processes

Next, we spell out the physical mechanisms underlying our model. We focus on surface relaxation, in the absence of growth. The steps move as a result of mass conservation under two main kinetic effects [2]: (i) the diffusion of adsorbed atoms (adatoms) on terraces, often simplified via the "quasi-steady approximation" by which adatom diffusion is supposed to equilibrate faster than steps move; and (ii) the atom attachment–detachment at steps. A variable entering this description is the (discrete) step chemical potential, which is a thermodynamic force equal to the variation of the step free energy with respect to the step positions. In our study, this energy accounts for entropic and nearest-neighbor elastic-dipole step–step interactions. Elements (i) and (ii) permeate the celebrated Burton–Cabrera–Frank (BCF) model [28].

By comparison to realistic material systems, this setting appears incomplete. For example, terrace diffusion anisotropies are not included. The dipole character of step–step interactions here does not fully describe long-range interactions that may be present, e.g., on the reconstructed Si(001). Diffusion of atoms along step edges, evaporation/condensation, desorption and external material deposition are left out.

In particular, a study of surface reconstructions that accounts for, e.g., the geometry of dimer rows with alternating orientations on adjacent terraces of Si(100) [29,17], would require an in-depth analysis of anisotropic effects in $2+1$ dimensions. Furthermore, the reconstruction generates internal stresses which may induce monopole–dipole step–step interactions [30]. This effect is of course not captured by the elastic-dipole model for steps used here [31].

In the spirit of the BCF theory [28], we assume that step motion occurs near thermodynamic equilibrium. This assumption is believed to be adequate for surface relaxation at macroscopic time scales. Material deposition from above and far-from-equilibrium kinetics are not touched upon here.

We expect that the present one-dimensional (1D) setting is, in a certain sense, minimal for surface reconstructions. Specifically, our formulation singles out issues intimately connected to averaging. We circumvent complications which may arise in a two-dimensional (2D) geometry or richer kinetics.

1.4. Macroscopic limit

We pass to the full continuum in the limit of vanishing step height, a, with fixed step density (surface slope). The ensuing variables of interest are treated as $\mathcal{O}(1)$, a-independent quantities. As in previous treatments of continuum limits for step flow, e.g., [5], the main macroscopic variables are the surface height, the adatom flux, and the continuum-scale step chemical potential.

Our analysis invokes certain simplifying hypotheses (and thus bears respective limitations) that are usually present in the study of continuum limits. Most notably, step trains are monotone and facets are absent. The step monotonicity simplifies the analysis, since the continuum limit is known to be questionable across peaks and valleys; furthermore, the height function, $h(x, t)$, is considered invertible in x for any fixed t. Microscale effects near facets are known to pose a challenging problem [32]. We assume that (appropriate) microscale averages of interest vary sufficiently slowly. The full continuum limit is assumed to exist rather than proved to exist. The latter task would require a rigorous study of (e.g., a priori estimates for) solutions to the discrete step flow.

We employ primarily formal arguments of classical homogenization [33] similarly to studies of diffusion in layered media [27]. Mathematical niceties such as issues of convergence [34], although necessary for a complete analytical understanding, lie beyond our present scope.

1.5. *Main results*

Next, we summarize our main results, which include: (i) Fick's law, which relates the large scale adatom flux, $\mathcal{J}^0(x,\tau)$, and step chemical potential $\mu(x,\tau)$, on the basis of adatom attachment–detachment boundary conditions at step edges; (ii) a conservation law for the macroscopic height profile, $h(x,\tau)$, from the step velocity law; and (iii) a variational formula for $\mu(x,\tau)$. The macroscopic time variable τ is discussed in Section 2.3. For notational economy, we omit the time (τ-) dependence unless we indicate otherwise.

1.5.1. *Adatom flux (Section 3.1)*

We will show that the macroscopic adatom flux is

$$\mathcal{J}^0(x,\tau) = -\mathcal{D}_e(x; m(x,\tau))\,\partial_x \varrho^{\mathrm{eq},0}(x,\tau). \tag{1}$$

In the above, $\varrho^{\mathrm{eq},0}$ is the continuum-scale version of the (discrete) equilibrium concentration, ρ_i^{eq}, at the ith step; and $\mathcal{D}_e$ is the effective parameter

$$\mathcal{D}_e(x; m(x)) = \frac{D^0(x)}{1 + q^0(x)\,m(x)}, \tag{2}$$

where D^0 is the average diffusivity

$$D^0(x) = \lim_{\substack{n_j\epsilon\downarrow 0\\ n_j\to\infty}} \overline{D}_j,$$

$$\overline{D}_j = \overline{D}_j^{\epsilon} = \left[\left(\frac{1}{y_{i_\circ} - y_{i_*}} \sum_{i\in I_j} \frac{y_{i+1}-y_i}{D_{i+1}(x)}\right)\right]^{-1}. \tag{3}$$

Here, $y_i = x_i/\epsilon$ where x_i is the i-th step position, D_i are microscale diffusivities, I_j is a set of integers expressing the mesoscale (see Section 2.2), and $\epsilon = a/\lambda$ (a: step height) where λ is a macroscopic length; $\tau = \epsilon^2 t$ (t: time). The q^0 is

$$q^0(x) = \frac{2D^0(x)}{k^0(x)}, \quad k^0(x) = \lim_{\substack{n_j\epsilon\to 0\\ n_j\to\infty}} (\epsilon\bar{k}_j),$$

$$\bar{k}_j(x) = 2\left\{\left[n_j^{-1}\sum_{i\in I_j}\left(\frac{1}{k_{\mathrm{u},i}} + \frac{1}{k_{\mathrm{d},i}}\right)\right]\right\}^{-1}, \tag{4}$$

where $k_{\mathrm{u},i}$ and $k_{\mathrm{d},i}$ are sticking rates for up- and down-step edges and the factor of 2 is included by convention; $k_{\mathrm{u},i}$ and $k_{\mathrm{d},i}$ are $\mathcal{O}(\epsilon^{-1})$ (see Remark 3). In (2), the variable m is defined as the (average) surface slope (cf. Remark 3)

$$m(x,\tau) = \lim_{\substack{n_j\epsilon\downarrow 0\\ n_j\to\infty}} \overline{m}_j(\tau),$$

$$\overline{m}_j = \left(n_j^{-1}\sum_{i\in I_j} m_i(\tau)^{-1}\right)^{-1} = \left(\frac{n_j\epsilon}{x_{i_\circ} - x_{i_*}}\right), \tag{5}$$

where $m_i(\tau) = \epsilon/w_i(\tau)$ and w_i is the ith terrace width. We use $x = x_i$ for some $i = i(j) \in I_j$; the choice of i becomes immaterial as $n_j\epsilon \downarrow 0$ (with $n_j \to \infty$).

Our derivation of (1) aims to clarify why the concentration entering Fick's law needs to be identified with $\varrho^{\mathrm{eq},0}$. This point was stated but not shown in [11]. Eqs. (1)–(5) are supplemented with the constitutive law [2]

$$\varrho^{\mathrm{eq},0}(x) = \rho_*[1 + \mu(x)/\vartheta], \tag{6}$$

where ϑ is the Boltzmann energy (absolute temperature in units of energy) and ρ_* is a positive constant.

1.6. *Adatom mass conservation (Section 3.2)*

We will establish the relation

$$m(x,\tau)u^0(x,\tau) + \partial_x\mathcal{J}^0(x,\tau) = 0, \tag{7}$$

where $u^0(x,\tau)$ denotes the continuum-scale step velocity (see Remark 4),

$$u^0(x,\tau) := \lim_{n_j\to\infty} \bar{u}_j,$$

$$\bar{u}_j = n_j^{-1}\sum_{i\in I_j} u_i, \quad u_i := \epsilon^{-2}v_i^{\epsilon}(t) = \mathrm{d}x_i^{\epsilon}/\mathrm{d}\tau, \tag{8}$$

and $m(x,\tau)$ is given by (5). We will show that

$$\partial_\tau h(x,\tau) = m(x,\tau)\,u^0(x,\tau) \quad (\tau = \epsilon^2 t), \tag{9}$$

which describes the motion of the effective level set for the graph $h(x,\tau)$. Thus, (7) becomes the familiar conservation law $\partial_t h + \Omega\partial_x\mathcal{J}^0 = 0$ ($\Omega = \epsilon^2$ is the atomic area).

1.7. *Chemical potential (Section 3.3)*

The fully continuum version of the step chemical potential is the variational derivative

$$\mu = \left(\frac{\delta\mathcal{E}[h]}{\delta h}\right)_{L^2}, \tag{10}$$

which is equivalent to the formula [5]

$$\dot{\mathcal{E}}(\tau) = \int_{\mathcal{U}} \mu(x,\tau)\,\partial_\tau h\,\mathrm{d}x, \tag{11}$$

where $\mathcal{U}$ expresses the relevant surface region. The functional $\mathcal{E}[h(\cdot,\tau)]$ is the large-scale surface free energy (continuum limit of the energy, E_N, of N steps)

$$\mathcal{E}[h(\cdot,\tau)] = \lim_{\epsilon\downarrow 0}(\epsilon E_N) = \frac{1}{3}\int_{\mathcal{U}} g^0(x,\tau)\,m(x,\tau)^3\,\mathrm{d}x. \tag{12}$$

The effective interaction parameter $g^0(x,\tau)$ is defined via (cf. Definition 6)

$$g^0(x,\tau) = \lim_{\substack{n_j\epsilon\downarrow 0\\ n_j\to\infty}} \bar{g}_j(\tau),$$

$$\bar{g}_j\overline{m}_j^2 := n_j^{-1}\sum_{i\in I_j}(3\breve{g}_i/2)m_i^2 \qquad (\breve{g}_i = \mathcal{O}(1)), \tag{13}$$

where $\breve{g}_i$ denotes the microscopic step–step interaction strength.

The second line of (12) forms a choice in accord with the elastic-dipole origin of the step interaction energy. Alternatively, it suffices to define $\mathcal{E}[h]$ as $\lim_{\epsilon\to 0}(\epsilon E_N)$ without resorting to the effective parameter g^0. In principle, g^0 depends on the surface slope, $m(x,\tau)$. In the special case with a non-composite stepped surface, by $\breve{g}_i = \breve{g} =$ const. we have $g^0(x) = 3\breve{g}/2$ provided the step densities squared, m_i^2, vary sufficiently slowly within each I_j, so that there is no difference between the mesoscale harmonic and arithmetic averages.

1.8. Organization and notation

The remainder of the paper is organized as follows. Section 2 offers an overview of the model, our assumptions and the homogenization formalism: we introduce the physical setting and formulate the equations of step motion (Section 2.1); introduce aspects of the relevant scales (Section 2.2); and briefly describe notions of homogenization (Section 2.3). In Section 3, we give details of the requisite multiscale expansions, order by order in perturbation, for 1 + 1 dimensions; and subsequently derive the desired evolution laws. In Section 4, we discuss our findings and pending issues, particularly notions of the weak formulation for homogenization and the case of 2 + 1 dimensions.

Throughout this paper, the terms 'full continuum limit', 'macroscale' and 'macroscopic limit' are used interchangeably. The time dependence is often (but not always) suppressed for notational economy. The symbol $Q^l(x,y)$, where l is an integer, denotes the coefficient of ϵ^l in the ϵ-perturbation expansion for Q. By $f = \mathcal{O}(g)$ we imply that $C_1 \le |f(z)/g(z)| \le C_2$ for some positive constants C_1 and C_2 as z approaches an extreme value. By $f = o(g)$ we mean that $|f(z)/g(z)| \downarrow 0$ as z approaches a given limit. The statement $\overline{Q}_j \to Q$ is used loosely to imply that, in the continuum limit, the average $\overline{Q}_j$ (over the jth mesoscale region) approaches Q.

2. Model and scale separation

Our goal with this section is to clarify the scale separation, and related concepts and notation needed in homogenization.

First, we describe the setting of steps and terraces in 1 + 1 dimensions. Second, we discuss the underlying scales. The smallest scale is the step height, a, and the largest scale is the size, λ, of the crystal sample. We define a mesoscale as an intermediate region of size d, $a \ll d \ll \lambda$. Third, we briefly review basic elements of classical homogenization.

2.1. Microscale model

The geometry consists of N steps descending in the positive x direction; see Fig. 1. We assume that all steps have the same height, a. The step positions are $x_i(t)$; $i = 0, \ldots, N-1$ and $N \gg 1$. Let $x_i(0) > x_{i-1}(0)$. The step ordering is assumed fixed for $t > 0$ because of the dipolar repulsive step interactions (see (19)). (A proof that the step ordering is preserved by the flow is feasible but not pursued here.) We conveniently apply screw periodic boundary conditions. To ensure that the surface slope is fixed, we set $w_i(t) := x_i(t) - x_{i-1}(t) = \mathcal{O}(a)$ for the ith-terrace width, w_i. By $x_{N-1}(0) - x_0(0) = \mathcal{O}(\lambda)$ for $N \gg 1$, we (initially) have

$$\sum_{i=1}^{N-1} w_i(0) = \mathcal{O}(Na) \quad \text{as } N \to \infty, \tag{14}$$

where the total length is $\lambda = Na = \mathcal{O}(1)$. Define $\epsilon = a/\lambda$ and set $\lambda = 1$.

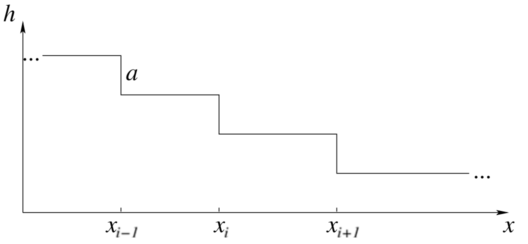

Fig. 1. Schematic (cross section) of steps with atomic height a and positions $x_i(t)$ in one spatial coordinate (x). The ith terrace is the region $\{x|x_{i-1} < x < x_i\}$.

Consider the ith terrace, $\mathcal{T}_{it} = \{x \mid x_{i-1}(t) < x < x_i(t)\}$, and let $U_t := \cup_{i=1}^{N} \mathcal{T}_{it}$, $|U_t| = \mathcal{O}(\lambda)$. The adatom concentration, $\rho_i(x,t) \equiv \rho_i^\epsilon(x,t)$, is defined via

$$\partial_x[D_i(x)\partial_x\rho_i] = \partial_t\rho_i \quad \text{for } x \in \mathcal{T}_{it}, \tag{15}$$

where $D_i = D_i^\epsilon$, $t \in (0,T]$ and $T = T^\epsilon$ is large enough to account for macroscopic observations (Section 2.3). Note that we do not apply the quasi-steady approximation, $\partial_t\rho_i \approx 0$, at this stage. Accordingly, (15) gives rise to convective terms in the overall flux of adatoms impinging on a step edge; cf. (17). The diffusivities $D_i(x)$ are positive and satisfy

$$0 < D_{\mathrm{m}} \le D_i(x) \le D_{\mathrm{M}} \quad \text{for } i = 0,\ 1, \ldots, N-1. \tag{16}$$

D_{m} and D_{M} are constants (independent of N).

Let $\varrho^\epsilon(\cdot,t)$ be the extension of the adatom concentration on $\mathcal{U} \supseteq \overline{U}_t$ ($\overline{U}_t$: closure of U_t) for all $t \ge 0$; e.g., $\mathcal{U} = [0,1]$. We must have $\varrho^\epsilon \equiv \rho_i^\epsilon$ for $x \in \mathcal{T}_{it}$ and all $t \ge 0$. Let us assume that $\varrho^\epsilon(\cdot,t)$ is C^2 (twice continuously differentiable in x) on U_t and bounded on $\mathcal{U}$. At each $x = x_i$ this ϱ^ϵ satisfies [28]

$$\mathcal{J}^\epsilon(x_i^-,t) - v_i\varrho^\epsilon(x_i^-,t) = k_{\mathrm{d},i}[\varrho^\epsilon(x_i^-,t) - \rho_i^{\mathrm{eq}}], \tag{17a}$$

$$-\mathcal{J}^\epsilon(x_i^+,t) + v_i\varrho^\epsilon(x_i^+,t) = k_{\mathrm{u},i}[\varrho^\epsilon(x_i^+,t) - \rho_i^{\mathrm{eq}}],$$

$$v_i = \mathrm{d}x_i/\mathrm{d}t. \tag{17b}$$

In the above, $Q(x_i^\pm)$ is the restriction of $Q(x)$ (where $Q = \mathcal{J},\ \varrho$) at $x = x_i$ from left ($-$) or right ($+$). The variable $\mathcal{J}^\epsilon(x,t)$ is the terrace adatom flux defined by Fick's law $\mathcal{J}^\epsilon(x,t) = -D_i^\epsilon(x)\partial_x\varrho^\epsilon(x,t)$ in $\mathcal{T}_{it}$; this is supplemented with the convective term $v_i\varrho^\epsilon$ at the step edge, where v_i is the step velocity. Note that $\mathcal{J}^\epsilon(\cdot,t)$ is C^1 (continuously differentiable) on U_t and bounded on $\mathcal{U}$, if $D_i(x) \in C^1(U_t)$. In (17), the parameters $k_{\ell,i}$ are positive kinetic attachment–detachment rates for an up- ($\ell = \mathrm{u}$) and a down- ($\ell = \mathrm{d}$) step edge, accounting for the Ehrlich–Schwoebel barrier [35,36].

Next, we describe ρ_i^{eq}, which incorporates step energies, in terms of $\{x_i\}_{i=0}^{N-1}$ [2]:

$$\rho_i^{\mathrm{eq}} = \rho_* e^{\mu_i/\vartheta} \sim \rho_*(1 + \mu_i/\vartheta), \quad |\mu_i| \ll \vartheta, \tag{18}$$

where μ_i is the step chemical potential (a thermodynamic force), and ρ_* is a given positive constant. In principle, we could have considered ρ_* as varying with i, replacing ρ_* by $\rho_{*,i} = \rho_* R_i$. Then, define $\tilde{\rho}_i := \rho_i/R_i$ and $\tilde{\rho}_i^{\mathrm{eq}} := \rho_i^{\mathrm{eq}}/R_i$. Because of linearity, the form of step equations (15), (17) and (22) remains intact; hence, drop the tildes and set $\rho_{*,i} = \rho_* =$ const.

The quantity μ_i expresses step–step repulsions. If steps interact entropically and as elastic dipoles, we have [2,31,37]

$$\mu_i = \frac{\delta E_N[\vec{x}]}{\delta x_i} = \epsilon^{-1}\left[\breve{g}_{i+1}\left(\frac{\epsilon}{w_{i+1}}\right)^3 - \breve{g}_i\left(\frac{\epsilon}{w_i}\right)^3\right],$$

$$\breve{g}_i = \mathcal{O}(1) > 0, \tag{19}$$

where $\vec{x} := (x_0, \ldots, x_{N-1})$, $E_N[\vec{x}]$ is the total step free energy,

$$E_N[\vec{x}] = \frac{1}{2}\sum_{i=1}^{N}\breve{g}_i\left(\frac{\epsilon}{x_i - x_{i-1}}\right)^2, \tag{20}$$

and the parameters $\breve{g}_i$ are strengths of the dipolar step–step interactions. Alternatively, μ_i can be defined through the formula [5]

$$\sum_{i=0}^{N-1} v_i \mu_i = \dot{E}_N \quad (\dot{E} := \mathrm{d}E/\mathrm{d}t), \tag{21}$$

where $v_i = \dot{x}_i$ is the ith-step velocity [5].

The last ingredient is the step velocity law, or mass conservation for adatoms:

$$\dot{x}_i = v_i = -(\Omega/\epsilon)[\mathcal{J}^{\epsilon,+} - \mathcal{J}^{\epsilon,-} - v_i \cdot (\varrho^{\epsilon,+} - \varrho^{\epsilon,-})]|_{x=x_i}, \tag{22}$$

where Ω is the atomic area and $Q^{\pm} := Q(x^{\pm})$; we henceforth set $\Omega = \epsilon^2$.

2.2. *Mesoscale*

The microscale material parameters introduced already are $\{D_i\}$, $\{k_{\mathrm{d},i}, k_{\mathrm{u},i}\}$, and $\{\breve{g}_i\}$. In this section, we define an intermediate scale, which facilitates the interpretation of averages emerging from homogenization (Section 3) and is consistent with the existence of the macroscopic limit. Averages of interest are invoked in general terms but left unspecified in this section.

The main physical idea is that material parameters can vary appreciably within numerous certain regions consisting of consecutive terraces. However, (appropriately defined) material averages over every such region vary slowly across many of these regions. The notion of the mesoscale helps express this idea. This statement is mathematically vague at the moment but points to a plausible, and appealing, view which we adopt: despite inhomogeneities at the microscale, the surface should appear homogeneous at a large enough scale.

2.2.1. *Some definitions*

Consider M sequences of (consecutive) steps in the step train, where $M \gg 1$ and $M = o(N)$ as $N \to \infty$. Let the jth sequence contain n_j steps labeled by $i \in I_j := \{i_*(j),\ i_*+1,\ \ldots,\ i_\circ(j)\}$ where $i_*(j) := \sum_{k=1}^{j-1} n_k$, $i_\circ(j) := \sum_{k=1}^{j} n_k - 1$ with $n_j \gg 1$ and $n_j = o(N)$ for $j = 1, \ldots, M$; and $i_*(1) := 0$, $i_\circ(M) = N - 1$. Each n_j is kept fixed, but the total length of corresponding terraces can vary by $o(n_j\epsilon)$ during evolution. All sequences in j are viewed as functions of x.

So far, we have not specified how the above sequences of steps are chosen. For this purpose, we resort to material parameter averages (to be determined in Section 3). For fixed ϵ, let the desired (i.e., harmonic, arithmetic or induced) average for every $\{\zeta_i^\epsilon\}_{i\in I_j}$ be denoted $\bar{\zeta}_j^\epsilon$; cf. Definition 6. To describe changes of these averages across I_j's, we define notions of slow variation.

Definition 1. (Discrete Version of Difference Quotient) The difference quotient of size $p \in \mathbb{Z} \setminus \{0\}$ for the sequence $\{\bar{\zeta}_j^\epsilon\}$ is

$$\delta^p \bar{\zeta}_j^\epsilon := \frac{\bar{\zeta}_{j+p}^\epsilon - \bar{\zeta}_j^\epsilon}{p}. \tag{23}$$

Define $\delta^0 \bar{\zeta}_j^\epsilon := 0$ *for definiteness.*

Definition 2. (Discrete Version of Slow Variation) The sequence $\{\bar{\zeta}_j^\epsilon\}_{j=1}^M$ is slowly varying if, for fixed and sufficiently small ϵ, there exist large integers $j_*(M) = o(M)$ and $j_\circ(M)$ with $M - j_\circ = o(M)$ such that, for every $j_* \le j \le j_\circ$,

$$\begin{aligned} &|p\delta^p \bar{\zeta}_j^\epsilon| = o(\bar{\zeta}_j^\epsilon) \quad \text{all } -p_* \le p \le p_\circ; \\ &M \gg 1 \ (0 < j - p_*,\ j + p_\circ < M), \end{aligned} \tag{24}$$

where $p_*(j), p_\circ(j) = o(M)$ and $n_j p_*, n_j p_\circ = o(N)$; $j_*, j_\circ, p_*, p_\circ \to \infty$ as $\epsilon \downarrow 0$.

The integers $j_*, j_\circ, p_*$ and $p_\circ$ in principle depend on ϵ; p_* and $p_\circ$ signify by how much one must shift j so that appreciable changes of the average $\bar{\zeta}_j^\epsilon$ occur. For any large (yet finite) M, these p_* and $p_\circ$ are small compared to M.

Remark 1. We henceforth assume that the sequence $\{I_j\}_{j=1}^M$, where $|I_j| = n_j = o(N) \gg 1$, is such that $\{\bar{\zeta}_j^\epsilon\}$ is slowly varying.

Definitions 1 and 2 allude to transferring averages to a continuum setting. Consider ϵ as small but finite; and replace the index j by the height variable $h = h_{i_*(j)}$. For a monotone step train, the variable h naturally corresponds to the step number, i, since the step height is constant; $h_i \sim h_0 - i\epsilon$. Accordingly, we introduce a (piecewise constant) function $\bar{\zeta}^\epsilon(h)$ such that $\bar{\zeta}^\epsilon(h_{i(j)}) = \bar{\zeta}_j^\epsilon$. We call such a $\bar{\zeta}^\epsilon(h)$ a 'continuous version' of $\bar{\zeta}_j^\epsilon$, assuming that, in the limit $n_j\epsilon \to 0$, $\bar{\zeta}^\epsilon(h)$ approaches a continuous function $\bar{\zeta}^0(h)$.

Definition 3. (Continuous Version of Difference Quotient) The *difference quotient* of size $\nu \in \mathbb{R} \setminus \{0\}$ for a continuous version $\bar{\zeta}^\epsilon(h)$ of $\{\bar{\zeta}_j^\epsilon\}$ is

$$\tilde{\delta}^\nu \bar{\zeta}^\epsilon(h) := \frac{\bar{\zeta}^\epsilon(h+\nu) - \bar{\zeta}^\epsilon(h)}{\nu}. \tag{25}$$

By direct analogy with Definition 2, we propose the following notion.

Definition 4. (Continuous Version of Slow Variation) The continuous version $\bar{\zeta}^\epsilon(h)$ is *slowly varying* if, for any $p = o(M)$ and $\nu = \nu(\epsilon) = \mathcal{O}(p\, n_j \epsilon) = o(1)$,

$$|\nu \tilde{\delta}^\nu \bar{\zeta}^\epsilon(h)| = o(\bar{\zeta}^\epsilon(h)) \quad \text{as } \epsilon \downarrow 0. \tag{26}$$

Eq. (24) or (26) implies $|\nu(\epsilon)\partial_h \bar{\zeta}^\epsilon(h)| \ll |\bar{\zeta}^\epsilon(h)|$; $\nu(\epsilon)$ expresses the height change across a few mesoscale regions. By assuming that the slow variation persists as $\epsilon \downarrow 0$ (or, $N \to \infty$), we pass to the full continuum limit, $\bar{\zeta}^\epsilon \to \bar{\zeta}^0 =: \zeta^0$. In the following, we use the x coordinate (as an independent variable) in place of h. By abusing notation, we write $\zeta^0(x)$ in place of $\zeta^0(h(x))$.

Remark 2. The slow variation is assumed to hold for averages of thermodynamic, kinetic and geometric variables, e.g., the step chemical potential, adatom flux, step velocity, and discrete slopes ϵ/w_i.

In light of the above discussion, we now define the concept of mesoscale.

Definition 5 (*Mesoscale*)**.** Recall Remark 1. Consider a given monotone step train, with $|I_j| = n_j \gg 1$, $n_j = o(N)$, $1 \le j \le M$ and $M, N \to \infty$. Assume $n_j/n_k = \mathcal{O}(1)$ for any j and k ($j \neq k$), and $n := \max_j\{n_j\}$. Any one of the M regions $\cup_{i\in I_j} \mathcal{T}_{(i+1)t}$ is called *the mesoscale*. Accordingly, a *mesoscale length* is any length L of the order of $d = n\epsilon$ with $\epsilon \ll L = \mathcal{O}(d) \ll 1 = \lambda$.

2.2.2. *Induced average*

At this point, it is advisable to introduce the induced average, a notion that helps link microscopic parameters to the continuum limit of the surface.

Definition 6. (Induced Average) Consider the function $f : \mathbb{R} \to \mathbb{R} \setminus \{0\}$ and averages $\{\bar{\zeta}_j^\epsilon\}_{j=1}^M$. The mesoscale average $\bar{\xi}_j^\epsilon$ of $\{\xi_i^\epsilon\}$ induced by $\{\zeta_i^\epsilon\}$ via f is

$$f(\bar{\zeta}_j^\epsilon)\, \bar{\xi}_j^\epsilon := n_j^{-1} \sum_{i\in I_j} f(\zeta_i^\epsilon)\xi_i^\epsilon; \quad j = 1, \ldots, M.$$

We use a bar on top of a symbol for both the starting ($\bar{\zeta}_j^\epsilon$) and the induced ($\bar{\xi}_j^\epsilon$) averages. These averages should be distinguished via the different symbols, ζ and ξ, for their variables. For our purposes, f can be thought of as Lipschitz continuous (see Appendix A).

2.3. Elements of homogenization

Next, we review formally some basics of classical homogenization theory, setting the technical framework for Section 3. We do not discuss aspects of two-scale convergence, keeping our exposition heuristic.

The fast spatial variable is $y := (x - \check{x})/\epsilon$ for some reference point $\check{x}$ (to be specified later). In view of diffusion equation (15), it is tempting to define fast and slow time variables as well, restricting attention to macroscopic times consistent with the quasi-steady approximation [2,5].

Definition 7. (Quasi-Steady Regime) For our purposes, the quasi-steady regime is characterized by times t such that $\tau = \epsilon^2 t = \mathcal{O}(1)$.

In Section 3, we show that Definition 7 yields evolution laws consistent with previous continuum limits. Recall the full-continuum conservation law for adatoms, $\partial_t h + \Omega\partial_x \mathcal{J}^0 = 0$ where h and $\mathcal{J}^0$ are the large-scale height and flux. By $\Omega = \epsilon^2$ and $\partial_x\mathcal{J}^0 = \mathcal{O}(1)$, we have $\partial_\tau h = \mathcal{O}(1)$ for $\tau = \epsilon^2 t$. Accordingly, we replace $\partial_t \to \partial_t + \epsilon^2\,\partial_\tau$, treating t and τ as independent. In the same vein, consider $T = T^\epsilon = \mathcal{O}(\epsilon^{-2})$ so that τ lies in a fixed interval. As $\epsilon \downarrow 0$, we claim that the dependent variables of interest settle to a steady state.

Remark 3. We take $n_j\epsilon \downarrow 0$ and $n_j \to \infty$ for $j = 1, 2 \ldots$. Consistent with other continuum treatments, e.g., [5], the following hypotheses are made.

(i) The step density (discrete slope) at the mesoscale is well defined, i.e.,

$$\frac{n_j\epsilon}{x_{i_\circ} - x_{i_*}} = \mathcal{O}(1) \quad \text{as } n_j\epsilon \downarrow 0,\ n_j \to \infty; \tag{27}$$

see Section 2.2 for definitions of $i_*(j)$ and $i_\circ(j)$. The left-hand side of (27) approaches the positive surface slope, $m(x) := |\partial_x h|$.

(ii) The height, h, chemical potential, μ_i, and flux, $\mathcal{J}$, are $\mathcal{O}(1)$ as $\epsilon \downarrow 0$.

(iii) The material parameters obey

$$k_{\ell,i}\epsilon,\ D_i,\ \breve{g}_i,\ \rho_*,\ \vartheta = \mathcal{O}(1) \quad \text{for all } i\ (\ell = \mathrm{u}, \mathrm{d}) \text{ as } \epsilon \downarrow 0.$$

In particular, steps move by "mixed kinetics", in which

$$\frac{D_i}{k_{\ell,i}\epsilon} = \mathcal{O}(1). \tag{28}$$

The next element to be discussed is the multiscale expansion. With regard to the concentration $\varrho^\epsilon(x,t)$ of Section 2.1, we write

$$\varrho^\epsilon(x,t) = \varrho^0(x,y,\tau,t) + \epsilon\,\varrho^1(x,y,\tau,t) + \epsilon^2\,\varrho^2(x,y,\tau,t) + o(\epsilon^2) \quad x \in \mathcal{U}. \tag{29}$$

To determine ϱ^l, it is necessary to apply dominant balance to (15) and enforce conditions (17). The multiscale expansion for the adatom flux $\mathcal{J}^\epsilon$ has the form

$$\mathcal{J}^\epsilon = \epsilon^{-1}\mathcal{J}^{(-1)}(x,y,\tau,t) + \mathcal{J}^0(x,y,\tau,t) + \epsilon\mathcal{J}^1(x,y,\tau,t) + o(\epsilon). \tag{30}$$

The solvability condition (to be invoked below) dictates that the coefficients ϱ^l in (29) be bounded in x and y, and do not grow as $n_j \to \infty$. Also, the coefficients $\mathcal{J}^l$ in expansion (30) for the flux should not grow with n_j.

Remark 4. In view of motion law (22) and Definition 7, we set $\mathrm{d}x_i/\mathrm{d}\tau = \mathcal{O}(1)$, and thereby infer that

$$v_i(t) = \epsilon^2\,(\mathrm{d}x_i/\mathrm{d}\tau) = \mathcal{O}(\epsilon^2). \tag{31}$$

This scaling with ϵ is consistent with the level set motion law $\partial_\tau h - u^0\partial_x h = 0$ for surfaces with the same parameters in all terraces, where $u^0(x,\tau) = \mathcal{O}(1)$ is the continuum limit of an appropriate average of $\epsilon^{-2}v_i$ and $m = \mathcal{O}(1)$.

3. Derivation of evolution laws

We proceed to derive the results presented in Section 1.5. We assert that boundary conditions (17), which suffice for the usual Fick's law, are decoupled from step velocity law (22) to the desired order of perturbation (at the chosen time scale). Further, we construct the continuum-scale chemical potential on the basis of (21) in terms of the step train free energy.

By recourse to (29) for $\tau = \mathcal{O}(1)$, we assume that each ϱ^l is stationary in the (fast) t and set $\partial_t\varrho^l \equiv 0$. By dominant balance, we find the following cascade:

$$\mathcal{O}(\epsilon^0):\ \partial_y^2\varrho^0 = 0, \tag{32a}$$

$$\mathcal{O}(\epsilon^1):\ \partial_y^2\varrho^1 + \partial_{yx}\varrho^0 + D_i(x)^{-1}\partial_x[D_i(x)\partial_y\varrho^0] = 0, \tag{32b}$$

$$\mathcal{O}(\epsilon^2):\ \partial_y^2\varrho^2 + \partial_{yx}\varrho^1 + D_i(x)^{-1}\partial_x[D_i(x)(\partial_y\varrho^1 + \partial_x\varrho^0)] = 0\ldots. \tag{32c}$$

These three equations suffice for identifying the macroscopic limit.

Our computations will involve steps and terraces that correspond to fixed I_j ($j = 1, \ldots, M$). Set $y = (x - \check{x})/\epsilon$ with $\check{x} = x_{i_*}$; thus, $y_{i_*} = 0$.

The possible dependence of $\varrho^l(x,y)$ on y may stem from kinetic conditions (17), imposed at the microscale boundaries y_i. By eliminating ρ_i^{eq}, we have

$$\varrho^+ - \varrho^- = -\epsilon\left(\frac{\mathcal{J}^-}{k_{\mathrm{d},i}\epsilon} + \frac{\mathcal{J}^+}{k_{\mathrm{u},i}\epsilon}\right) + \epsilon v_i\left(\frac{\varrho^-}{k_{\mathrm{d},i}\epsilon} + \frac{\varrho^+}{k_{\mathrm{u},i}\epsilon}\right) \quad y = y_i. \tag{33}$$

3.1. Fick's law

In this subsection, we derive (1)–(5).

Since $x_i(t) = x_i^\epsilon(t)$ are moving boundaries, or Lagrangian coordinates, we expand

$$x_i = x_i^0 + \epsilon x_i^1 + o(\epsilon). \tag{34}$$

By Remark 4 and expansion (30) for the flux, the step velocity law (22) reads

$$v_i^\epsilon(t) = \epsilon^2[u_i(\tau) + o(1)] = (\mathcal{J}^{(-1),-} - \mathcal{J}^{(-1),+}) + o(1), \quad y = y_i, \tag{35}$$

where $u_i(\tau) = \mathcal{O}(1)$ and $\mathcal{J}^{(-1),\pm}$ is the restriction of the leading-order flux term $\mathcal{J}^{(-1)}(x,y)$ at $y = y_i^0$ from left ($-$) or right ($+$). In (35), we leave the step number dependence (via i) in the leading-order term for v_i^ϵ. To the lowest order in perturbation, the adatom flux is continuous across step edges, $\mathcal{J}^{(-1),+} = \mathcal{J}^{(-1),-}$. In fact, this property can be extended to the next higher order, as shown below.

3.1.1. Lowest (zeroth) order

First, consider (32a). The solution reads

$$\varrho^0(x,y) = A_i(x)y + B_i(x) \quad y_{i-1}^0 < y < y_i^0\ (i \in I_j), \tag{36}$$

where A_i and B_i are viewed as $\mathcal{O}(1)$ integration constants, to be found via boundary conditions at step edges. By virtue of (35), we obtain

$$\epsilon\mathcal{J}(x) \to \mathcal{J}^{(-1)}(x,y) = -D_i(x)\partial_y\varrho^0(x,y) = -D_i(x)A_i(x), \tag{37}$$

where $y_{i-1}^0 < y < y_i^0$. Thus, the continuity of flux to this order yields

$$D_iA_i = D_{i-1}A_{i-1} = \cdots = D_{i_*}A_{i_*} \Rightarrow A_i(x) = \frac{D_{i_*}(x)}{D_i(x)} A_{i_*}(x). \tag{38}$$

The dominant balance of conditions (33) and (36) entail

$$(A_{i+1} - A_i)y_i^0 + B_{i+1} - B_i = \left(\frac{D_i}{k_{\mathrm{u},i}\epsilon} + \frac{D_i}{k_{\mathrm{d},i}\epsilon} \right) A_i.$$

To obtain B_i, we add up the last equations backwards in i in terms of a telescopic sum. The result reads

$$B_i = B_{i_*} + A_{i_*}D_{i_*} \times \left[-\frac{y_i^0}{D_i} + \sum_{p=i_*}^{i-1} \left(\frac{y_{p+1} - y_p}{D_{p+1}} + \sum_{\ell=\mathrm{u,d}} \frac{2}{k_{\ell,p}\epsilon} \right) \right], \tag{39}$$

where $i \in I_j$ and $i > i_*$. By (36), (38) and (39), we find

$$\varrho^0(x, y) = \frac{D_{i_*}(x)A_{i_*}(x)}{D_i(x)} (y - y_i^0) + B_{i_*}(x) + D_{i_*}(x)A_{i_*}(x) \sum_{p=i_*}^{i-1} \left(\frac{y_{p+1}^0 - y_p^0}{D_{p+1}(x)} + \sum_{\ell=\mathrm{u,d}} \frac{2}{k_{\ell,p}\epsilon} \right). \tag{40}$$

By (16), which exacts the bounds for $D_i(x)$, we assert that

$$0 < \frac{y_i^0 - y_{i_*}^0}{D_M} \le \sum_{p=i_*}^{i-1} \frac{y_{p+1}^0 - y_p^0}{D_{p+1}(x)} \le \frac{y_i^0 - y_{i_*}^0}{D_m}, \tag{41}$$

where $y_i^0 - y_{i_*}^0 = \mathcal{O}(n_j)$ for large enough i in I_j. Hence, the sums in (40) diverge as $n_j \to \infty$ with $i = i_\circ$ and the solvability condition is not satisfied *unless* $A_{i_*}(x) \equiv 0$. Thus, we reach the following, anticipated result [11].

Proposition 1. *The zeroth-order adatom concentration is*

$$\varrho^0(x, y) = B_{i_*}(x) = B(x), \tag{42}$$

independent of the fast variable. The corresponding flux is $\mathcal{J}^{(-1)}(x, y) \equiv 0$.

3.1.2. First order

In order to obtain a relation between $\mathcal{J}^0$ and $B(x)$, we proceed to computing the next-order adatom coefficient, $\rho^1(x, y)$. By (32b) and Proposition 1, we readily obtain

$$\varrho^1(x, y) = C_i(x)y + F_i(x) \quad y_{i-1}^0 + \epsilon y_{i-1}^1 < y < y_i^0 + \epsilon\, y_i^1, \tag{43}$$

suppressing the time variable, τ. Thus, the adatom concentration up to $\mathcal{O}(\epsilon)$ is $B(x) + \epsilon[C_i(x)y + F_i(x)]$. The corresponding terrace adatom flux reads

$$\mathcal{J}^0(x, y) = -D_i(x)[C_i(x) + \partial_x B(x)] \quad (y_{i-1}^0 + \epsilon y_{i-1}^1 < y < y_i^0 + \epsilon\, y_i^1). \tag{44}$$

By dominant balance applied to velocity law (22) under expansion (35), we readily verify the following remark.

Remark 5. The adatom flux $\mathcal{J}^0(x, \cdot)$ is continuous across step edges.

Thus, by enforcing the continuity of $\mathcal{J}^0(x, y)$ at each boundary $y = y_i$ we get

$$D_i(x)[C_i(x) + \partial_x B(x)] = D_{i+1}(x)[C_{i+1}(x) + \partial_x B(x)] \Rightarrow C_i(x) = \frac{D_{i_*}(x)}{D_i(x)}[C_{i_*}(x) + \partial_x B] - \partial_x B \quad (i,\ i+1 \in I_j). \tag{45}$$

We turn attention to boundary conditions (33). These are recast to the form

$$[C_{i+1}(x) - C_i(x)](y_i^0 + \epsilon y_i^1) + F_{i+1}(x) - F_i(x) + \mathcal{O}(\epsilon) = \left(\frac{D_i}{k_{\mathrm{d},i}\epsilon} + \frac{D_i}{k_{\mathrm{u},i}\epsilon} \right) [C_i(x) + \partial_x B(x)] + \mathcal{O}(\epsilon) \quad (i, i+1 \in I_j). \tag{46}$$

Thus, by Remark 3, the correction terms ϵy_i^1 do not contribute to this order. By using (45) and summing up (46) via a telescopic sum, we obtain

$$F_i(x) = F_{i_*}(x) + D_{i_*}(x)[C_{i_*}(x) + \partial_x B] \times \left[\sum_{p=i_*}^{i-1} \left(\sum_{\ell=u,d} \frac{1}{k_{\ell,p}\epsilon} + \frac{y_{p+1} - y_p}{D_{p+1}} \right) - \frac{y_i}{D_i} \right]. \tag{47}$$

The substitution of (45) and (47) into (43) yields

$$\varrho^1(x, y) = \left(\frac{D_{i_*}(x)}{D_i(x)}[C_{i_*}(x) + \partial_x B(x)] - \partial_x B \right) (y - y_i^0) + F_{i_*}(x) + y_i^0 \left\{ -\partial_x B + D_{i_*}(x)[C_{i_*}(x) + \partial_x B](y_i^0)^{-1} \times \sum_{p=i_*}^{i-1} \left(\frac{y_{p+1}^0 - y_p^0}{D_{p+1}(x)} + \sum_{\ell=u,d} \frac{2}{k_{\ell,p}\epsilon} \right) \right\} \tag{48}$$

where $y_{i-1}^0 + \epsilon y_{i-1}^1 < y < y_i^0 + \epsilon y_i^1$ and $i > i_*$. By requiring that ϱ^1 be bounded as i increases, we impose the necessary condition that the coefficient of y_i^0 vanish when $i - i_* = \mathcal{O}(n_j) \to \infty$ in (48). By $i = i_\circ(j)$, we thus find

$$D_{i_*}(x)[C_{i_*}(x) + \partial_x B] \lim_{\substack{n_j \to \infty \\ n_j\epsilon \downarrow 0}} \left[\frac{1}{y_{i_\circ}^0} \sum_{p \in I_j} \left(\sum_{\ell=u,d} \frac{2}{k_{\ell,p}\epsilon} + \frac{y_{p+1}^0 - y_p^0}{D_{p+1}} \right) \right] = \partial_x B. \tag{49}$$

By definitions (3) and (4), this relation is recast to the form

$$D_{i_*}(x)[C_{i_*}(x) + \partial_x B] \left[1 + q^0(x) \lim_{\substack{n_j \to \infty \\ n_j\epsilon \downarrow 0}} \frac{n_j\epsilon}{x_{i_\circ} - x_{i_*}} \right] = D^0(x)\partial_x B,$$

where the requisite limit is the surface slope (see Remark 3); thus,

$$D_{i_*}(x)[C_{i_*}(x) + \partial_x B(x)] = \frac{D^0(x)}{1 + q^0(x)m(x)} \partial_x B. \tag{50}$$

Eq. (50) entails the desired Fick's law. By (44) and (45), the flux is [11]

$$\mathcal{J}^0(x, y) = -D_{i_*}(x)[C_{i_*}(x) + \partial_x B(x)].$$

Proposition 2. *The macroscopic limit of the adatom flux reads*

$$\mathcal{J}^0(x) = -\frac{D^0(x)}{1 + q^0(x)m(x)} \partial_x B, \tag{51}$$

where D^0 and q^0 are defined in (3) and (4); see Section 3.1.3 for $B(x)$.

3.1.3. *Equilibrium concentration*

Next, we show that the $B(x)$ in (51) can be identified with the continuum-scale version, $\varrho^{\mathrm{eq},0}$, of ρ_i^{eq}, which is affine in the large-scale chemical potential, μ. For this purpose, we revisit kinetic conditions (17). By adding up these equations, we obtain the relation

$$\epsilon\left(\frac{\mathcal{J}^-}{k_{\mathrm{d},i}\epsilon}-\frac{\mathcal{J}^+}{k_{\mathrm{u},i}\epsilon}\right)+\epsilon v_i\left(\frac{\varrho^+}{k_{\mathrm{u},i}\epsilon}-\frac{\varrho^-}{k_{\mathrm{d},i}\epsilon}\right)=(\varrho^++\varrho^-)|_{y_i} - 2\rho_i^{\mathrm{eq}}. \tag{52}$$

By $k_{\ell,i}\epsilon = \mathcal{O}(1)$ (Remark 3), the first term is $\mathcal{O}(\epsilon)$; and, in view of Remark 4, the second term is $\mathcal{O}(\epsilon^3)$. Thus, by formally writing $\rho_i^{\mathrm{eq}} = \varrho^{\mathrm{eq},0}(x,y)+o(1)$, we apply the usual dominant-balance argument to order $\mathcal{O}(\epsilon^0)$ and (42) to infer

$$2\varrho^0=\varrho^{0,+}+\varrho^{0,-}=2\varrho^{\mathrm{eq},0}. \tag{53}$$

Proposition 2 and (53) yield formulas (1)–(5). By $\mu_i=\mu(x)+o(1)$ and (18), we express $\varrho^{\mathrm{eq},0}$ in terms of μ, winding up with (6).

3.2. *Mass conservation and level set motion laws*

In this subsection, we derive Eqs. (7) and (8) with recourse to step velocity law (22). This law involves a jump of the flux, $\mathcal{J}(x,\cdot)$, at each step edge ($y = y_i$). Recall that the flux is continuous to the first two orders in ϵ. The jump is revealed to the next higher order. We follow two alternate routes. One method is to apply the solvability condition (in the context of homogenization) in the spirit of Section 3.1. Another route is a weak formulation [5]. Further, we derive level set motion law (9), which introduces the time derivative $\partial_\tau h$.

3.2.1. *Perturbation expansion*

We continue the argument of Section 3.1. In summary, we resort to (32c), solve for $\varrho^2(x,y)$ and $\mathcal{J}^1$, and determine the discontinuity of $\mathcal{J}$ at each step edge up to order $\mathcal{O}(\epsilon)$. The solvability condition for $\mathcal{J}^1$ yields the desired formula.

Eq. (32c) along with Proposition 2 and (2) yield

$$\begin{aligned}\partial_y[D_i(x)\partial_y\varrho^2(x,y)] &= -\partial_x\{D_{i_*}(x)[C_{i_*}(x)+\partial_xB]\}\\ &\quad -D_i(x)\partial_xC_i \Rightarrow \varrho^2(x,y)\\ &= yG_i(x)+H_i(x)-\{\partial_xC_i\\ &\quad +D_i(x)^{-1}\partial_x[\mathcal{D}_{\mathrm{e}}(x)\partial_xB]\}\frac{y^2}{2}.\end{aligned} \tag{54}$$

The adatom concentration on the ith terrace up to $\mathcal{O}(\epsilon^2)$ reads

$$\begin{aligned}\varrho(x,y) &= \varrho^0(x,y)+\epsilon\varrho^1(x,y)+\epsilon^2\varrho^2(x,y)+o(\epsilon^2)\\ &= B(x)+\epsilon[C_i(x)y+F_i(x)]+\epsilon^2\{yG_i(x)+H_i(x)\\ &\quad -[\partial_xC_i+D_i(x)^{-1}\partial_x(\mathcal{D}_{\mathrm{e}}(x)\partial_xB)]y^2/2\}+o(\epsilon^2).\end{aligned} \tag{55}$$

The respective surface flux on the ith terrace is

$$\begin{aligned}\mathcal{J}(x,y) &= -D_i(x)[(\partial_y\varrho^1+\partial_x\varrho^0)+\epsilon(\partial_y\varrho^2+\partial_x\varrho^1)]+o(\epsilon)\\ &= -D_i(x)[C_i(x)+\partial_xB]-\epsilon\{D_i(x)[G_i(x)+\partial_xF_i]\\ &\quad -y\partial_x(\mathcal{D}_{\mathrm{e}}(x)\partial_xB)\}+o(\epsilon).\end{aligned} \tag{56}$$

The $\mathcal{O}(\epsilon^0)$ term is of course continuous at each y_i^0. At $y = y_i^0$ this flux obeys

$$\begin{aligned}\epsilon(\mathcal{J}^{1,+}-\mathcal{J}^{1,-}) &= -\epsilon[D_{i+1}(x)(G_{i+1}(x)+\partial_xF_{i+1})\\ &\quad -D_i(x)(G_i(x)+\partial_xF_i)].\end{aligned}$$

The next task is to determine the coefficient $G_i(x)$. By virtue of (35), step velocity law (22) with $\Omega = \epsilon^2$ is recast to the form

$$u_i+o(1)=-[\mathcal{J}^{1,+}-\mathcal{J}^{1,-}+o(1)]+\epsilon^2u_i\,[\varrho^{1,+}-\varrho^{1,-}+o(1)]$$
$$y=y_i.$$

The convective term on the right-hand side of this equation does not contribute to the lowest order. Thus, we obtain the distinguished limit

$$\begin{aligned}u_i &= -(\mathcal{J}^{1,+}-\mathcal{J}^{1,-})|_{y_i^0} \Rightarrow u_i = D_{i+1}(G_{i+1}+\partial_xF_{i+1})\\ &\quad -D_i(G_i+\partial_xF_i).\end{aligned} \tag{57}$$

This result amounts to mass conservation: the jump in the flux is balanced by the step velocity. The convective terms do not contribute because of the slow time scale. (57) leads to a telescopic sum for G_i, which yields

$$\begin{aligned}G_i(x) &= \frac{D_{i_*}(x)}{D_i(x)}[G_{i_*}(x)+\partial_xF_{i_*}(x)]\\ &\quad -\partial_xF_{i_*}+D_i(x)^{-1}\sum_{p=i_*}^{i-1}u_p.\end{aligned} \tag{58}$$

By (56) and (58), the coefficient of the $\mathcal{O}(\epsilon)$ term for the flux reads

$$\begin{aligned}\mathcal{J}^1(x,y) &= -D_{i_*}(x)[G_{i_*}(x)+\partial_xF_{i_*}(x)]\\ &\quad +(y-y_i^0)\partial_x(\mathcal{D}_{\mathrm{e}}(x)\partial_xB)\\ &\quad +y_i^0\left[\partial_x(\mathcal{D}_{\mathrm{e}}\partial_xB)-(y_i^0)^{-1}\sum_{p=i_*}^{i-1}u_p\right].\end{aligned} \tag{59}$$

Now let $i = i_\circ(j) = i_*(j)+n_j-1$. By requiring that $\mathcal{J}^1$ does *not* grow as $n_j \to \infty$ (imposing the solvability condition), we assert that

$$\begin{aligned}\partial_x(\mathcal{D}_{\mathrm{e}}(x)\partial_xB) &= \lim_{\substack{n_j\to\infty\\ n_j\epsilon\to 0}}\left[\left(\frac{n_j}{y_{i_\circ(j)}^0}\right)\left(n_j^{-1}\sum_{p=i_*}^{i_\circ}u_p\right)\right]\\ &\Rightarrow -\partial_x\mathcal{J}^0(x)=m(x)\,\bar{u}(x).\end{aligned}$$

Proposition 3. *The macroscopic limit, $\mathcal{J}^0$, of the surface flux obeys (7), where the continuum-scale step velocity is the arithmetic mean (8).*

3.2.2. *Weak formulation for mass conservation*

Following [5], we write step velocity law (22) in the form

$$\epsilon^2u_i=-\epsilon\,[\mathcal{J}+\mathcal{O}(\epsilon^2)]_i;\qquad [Q]_i := Q(y_i^+)-Q(y_i^-). \tag{60}$$

Now multiply both sides of (60) by a test function, ϕ_i, that is constant on each mesoscale region and sum over i to obtain

$$\begin{aligned}\epsilon\sum_{i=0}^{N-1}\phi_iu_i &= -\sum_{i=0}^{N-1}[\mathcal{J}]_i\phi_i+\mathcal{O}(\epsilon)\\ &\Rightarrow \sum_j(n_j\epsilon)\phi_{i_*(j)}\left(n_j^{-1}\sum_{i\in I_j}u_i\right)\\ &= -\sum_j\phi_{i_*(j)}\sum_{i\in I_j}[\mathcal{J}]_i+o(1)\\ &\Rightarrow \sum_j(n_j\epsilon)\phi_{i_*(j)}\bar{u}_j=-\sum_j\phi_{i_*(j)}\sum_{i\in I_j}[\mathcal{J}]_i+o(1)\\ &\Rightarrow \int\phi(x)\,u^0(x)m(x)\,\mathrm{d}x\\ &= -\int\phi(x)\,\mathrm{d}\mathcal{J}^0(x)\quad \text{as } \epsilon\downarrow 0,\ n_j\epsilon\downarrow 0.\end{aligned} \tag{61}$$

This implies (7) in the weak sense.

3.2.3. Level set motion law

Next, we derive geometric law (9) with recourse to a weak formulation. For this purpose, define

$$\Im_N := \epsilon \int_0^{T_0} \sum_i u_i \phi_i \, \mathrm{d}\tau; \quad u_i = \mathrm{d}x_i/\mathrm{d}\tau, \tag{62}$$

where the sequence $\{\phi_i\}$ consists of smooth, compactly supported functions $\phi_i : (0, T_0] \to \mathbb{R}$. We will show that, in the continuum limit,

$$\int_0^{T_0} \int \phi \, h_\tau \, \mathrm{d}x\mathrm{d}\tau = \int_0^{T_0} \int \phi \, u^0 \, m \, \mathrm{d}x\mathrm{d}\tau, \tag{63}$$

for any smooth test function $\phi : \mathcal{U} \times (0, T_0] \to \mathbb{R}$ where ϕ is compactly supported; we can choose $\phi_i(\tau) = \phi(x_i, \tau)$. Note that u^0 denotes the macroscopic limit of $\bar{u} = n_j^{-1} \sum_{i \in I_j} u_i$, and $h_\tau := \partial_\tau h$.

First, consider the case with homogeneous steps and terraces, i.e., when the material parameters remain unchanged across terraces. By (62), we have

$$\Im_N \to \int_0^{T_0} \int u^0 \, \phi \, \mathrm{d}h\mathrm{d}\tau = \int_0^{T_0} \int u^0 \, m \, \phi \, \mathrm{d}x\mathrm{d}\tau$$
$$\text{as } N \to \infty, \qquad N\epsilon = \mathcal{O}(1), \tag{64}$$

where u^0 is the continuum limit of $\{u_i\}$.

On the other hand, by integration by parts, we assert that

$$\begin{aligned} \Im_N &= -\epsilon \int_0^{T_0} \sum_i x_i \frac{\mathrm{d}\phi_i}{\mathrm{d}\tau} \, \mathrm{d}\tau \\ &\to -\int_0^{T_0} \int x \, (\phi_\tau|_h) \, m \, \mathrm{d}x\mathrm{d}\tau, \end{aligned} \tag{65}$$

where $\phi_\tau|_h$ is the partial derivative of ϕ with respect to τ with *fixed* h. By passing from Lagrangian to Eulerian coordinates, write $\phi_\tau|_h = \phi_\tau|_x - \phi_x \, (h_\tau/h_x)$ where $h_x = -m < 0$. By integration by parts in τ and in x, (65) yields

$$\begin{aligned} \Im_N &\to -\int_0^{T_0} \int x h_{x\tau} \phi \, \mathrm{d}x\mathrm{d}\tau - \int_0^{T_0} \int x \phi_x h_\tau \, \mathrm{d}x\mathrm{d}\tau \\ &= \int_0^{T_0} \int [(x\phi)_x - x\phi_x] h_\tau \, \mathrm{d}x\mathrm{d}\tau. \end{aligned} \tag{66}$$

The comparison of (64) and (66) implies (63).

Alternatively, for the above case of a non-composite stepped surface, write $h(x_i(t), t) = \text{const.}$ for each terrace (level set of h). The differentiation of this equation with respect to t yields the desired law in the continuum limit [5].

In the case of a composite stepped surface, we need to slightly modify the manipulation of sum $\Im_N$ in (64) and (65). In particular, for appropriate test sequences, we use the notion of induced average (Definition 6) and hence write

$$\begin{aligned} \Im_N &= \int_0^{T_0} \sum_{j=1}^{M} (n_j\epsilon) \phi_{i_*(j)} \left(n_j^{-1} \sum_{i \in I_j} u_i \right) \mathrm{d}\tau \\ &\to \int_0^{T_0} \int \phi \, u^0 \, \mathrm{d}h\mathrm{d}\tau, \end{aligned} \tag{67}$$

where ϕ_i is constant on each mesoscale region. On the other hand, $\Im_N$ equals

$$\begin{aligned} \Im_N &= \int_0^{T_0} \sum_{j=1}^{M} (n_j\epsilon) \phi_j \left(n_j^{-1} \sum_{i \in I_j} \frac{\mathrm{d}x_i}{\mathrm{d}\tau} \right) \mathrm{d}\tau \\ &= -\int_0^{T_0} \sum_{j=1}^{M} (n_j\epsilon) \frac{\mathrm{d}\phi_j}{\mathrm{d}\tau} \left(n_j^{-1} \sum_{i \in I_j} x_i \right) \mathrm{d}\tau \\ &\to -\int_0^{T_0} \int (\phi_\tau|_h) x \, \mathrm{d}h\mathrm{d}t. \end{aligned} \tag{68}$$

The remainder of the derivation leading to (63) follows directly from (66).

3.3. Step chemical potential and free energy

Next, we focus on the derivation of (10)–(13). To obtain the continuum-scale chemical potential, μ, in terms of $\mathcal{E} = \lim_{\epsilon \to 0}(\epsilon E_N)$, we use (21). By $\tau = \epsilon^2 t$ and $u_i = \epsilon^{-2} v_i + o(1)$, we have

$$\begin{aligned} \epsilon \frac{\mathrm{d}E_N}{\mathrm{d}\tau} &= \epsilon \sum_{i=0}^{N-1} u_i \mu_i = \sum_{j=1}^{M} (n_j\epsilon) \left(n_j^{-1} \sum_{i \in I_j} u_i \mu_i \right) \\ &= \sum_{j=1}^{M} (n_j\epsilon) \bar{u}_j \bar{\mu}_j \Rightarrow \dot{\mathcal{E}}(\tau) \\ &= \int u^0(x, \tau) \, \mu(x, \tau) \, \mathrm{d}h \quad \text{as } n_j \to \infty, \ n_j\epsilon \downarrow 0. \end{aligned} \tag{69}$$

The rightmost-hand side of the first line in (69) serves as the definition of $\bar{\mu}_j$.

Recall the free energy E_N given by (20). To make a connection to the continuum-scale free energy of a non-composite stepped surface [38,2], we use an induced average of $\{\breve{g}_i\}$. By Definition 6, we obtain

$$\begin{aligned} \epsilon E_N(t) &= \frac{\epsilon}{2} \sum_{j=1}^{M} \sum_{i \in I_j} \breve{g}_i m_i^2 = \frac{1}{3} \sum_{j=1}^{M} (n_j\epsilon) \bar{g}_j \, \bar{m}_j^2 \\ &\to \frac{1}{3} \int g^0(x, \tau) \, m(x, \tau)^2 \, \mathrm{d}h =: \mathcal{E}(\tau) \quad \text{as } \epsilon \downarrow 0, \end{aligned} \tag{70}$$

if the average $\bar{g}_j$ varies slowly across mesoscale regions. Eq. (12) ensues.

4. Discussion and conclusion

We formally studied the consistency of macroscopic laws for crystal surface relaxation with the discrete step flow when terraces and steps are characterized by sequences of distinct material parameters. We assume that an intermediate scale, the mesoscale, links the slow spatial variation of microscale averages to the property that the crystal surface appears homogeneous at the macroscale.

Our methodology relies on classical homogenization, by which the adatom concentration and mass flux are globally expressed in terms of multiscale expansions. Two features of these expansions are: (i) step boundaries, included through boundary conditions at the fast spatial variable [27]; and (ii) a macroscopic time scale consistent with the quasi-steady approach.

The form of macroscopic laws is found to be the same as in the case of a non-composite stepped surface [7,9]. These laws comprise Fick's law of surface diffusion (with an appropriate mobility), the mass conservation statement for the surface height, and a variational formula for the chemical potential; see Propositions 1–3. The homogenization approach shows *how* the large-scale surface mobility turns out to be a function of the slope, with the effective diffusivity and kinetic rate given as appropriate harmonic averages. The dependence of the mobility on the slope, emerging from the solvability condition, is viewed as a result conceptually *distinct* from the electric-circuit analog of a stepped surface [6].

Regarding the large-scale chemical potential, μ, we assumed that the discrete step free energy has a continuum limit; and expressed this limit in terms of the induced average of microscale parameters for step–step interactions.

Our work leaves several unresolved questions. Next, we make an attempt to single out and discuss two of such issues, namely, the rigorous derivation of homogenized equations via a weak formulation, even in $1+1$ dimensions; and the nature and derivation of effective laws in full $2+1$ dimensions (in non-radial geometries).

4.1. On the rigorous derivation of homogenized equations

We deem that a rigorous study of homogenization of step dynamics is a challenging problem. To start with, finding the appropriate Hilbert space for a weak formulation is nontrivial. The difficulty stems from the simultaneous presence of (i) step motion *and* (ii) discontinuity of adatom concentration at each step. Suppose that we simplify the problem, considering the system in equilibrium (time-independent case); then, issue (i) disappears. We may use the Hilbert space $H = \prod_i H^1([x_{i-1}, x_i])$ for a weak formulation and prove the existence of a unique solution at the microscale where H^1 is a well-known Sobolev space. The weak formulation reads

$$\begin{aligned}\sum_i \int_{[x_{i-1},x_i]} & D_i^\epsilon \nabla\rho^\epsilon \nabla\varphi\, dx \\ &+ \sum_i [k_i((\rho_{i-1}^+ - \rho_i^{eq})\varphi^+ + (\rho_i^- - \rho_i^{eq})\varphi^-)]_{x=x_i} \\ =& \int_{\mathcal{U}} F\,\varphi\, dx, \end{aligned} \tag{71}$$

where $\mathcal{U}$ is time-independent, φ is a test function, and F denotes a deposition flux (included for completeness). It is tempting to claim that the homogenization procedure can be carried out via this formulation. In the time-dependent case, however, the step position x_i depends on t and the domain division cannot be made independent of time. Thus, a global weak solution in the sense of [12,13,39] seems to provide a more appropriate working framework. However, finding a Hilbert space for such a weak formulation is difficult due to issue (ii) mentioned above. Work in this direction is in progress.

4.2. Macroscopic limit in $2+1$ dimensions

In $2+1$ dimensions the classical homogenization of this paper is not directly applicable because explicit solutions to the diffusion equation are in principle intractable. A plausible way to circumvent this difficulty is to invoke approximate solutions for slowly varying step trains in the spirit of [5]. However, care should be exercised; a naive application of such approximations may lead to an erroneous calculation of the flux component that is parallel to step edges.

More generally, homogenization in a two-dimensional setting is different from its one-dimensional counterpart. Because of the existence of two flux components, parallel and perpendicular to steps, the corresponding averages may be distinctly different. For instance, if we consider a periodic $(2+1)$-dimensional setting, we expect that the macroscopic Fick's law has the (vector) form (cf. [5])

$$\mathbf{J} = -\begin{pmatrix} \mathcal{D}_{\mathrm{av}}^{\perp}(1+q^0\, m)^{-1} & 0 \\ 0 & \mathcal{D}_{\mathrm{av}}^{\parallel} \end{pmatrix} \begin{pmatrix} \partial_\perp \mu \\ \partial_\parallel \mu \end{pmatrix},$$

in a local coordinate system relative to step edges, where $\mathcal{D}_{\mathrm{av}}^{\perp}$ and $\mathcal{D}_{\mathrm{av}}^{\parallel}$ possibly involve harmonic and arithmetic averages of terrace diffusivities, $q^0 \propto 2\mathcal{D}_{\mathrm{av}}^{\perp}/k^0$, and k^0 stems from a direct extension of (4). The above formula for the vector-valued, large-scale flux $\mathbf{J}$ forms a conjecture. We are less familiar with the homogenized limit of Fick's law in a non-periodic setting; this limit should of course depend on assumptions about the microscopic parameters. We anticipate that the remaining evolution laws (other than Fick's law) in $2+1$ dimensions should be similar in form to their $(1+1)$-dimensional versions.

Acknowledgments

The authors have benefited from discussions with Professors Robert V. Kohn, Athanasios E. Tzavaras and John D. Weeks. The authors' research was supported by NSF DMS0847587 at the University of Maryland. The second author's (KN) research was also supported by a Graduate Student Summer Research Fellowship at the University of Maryland during the summer of 2011.

Appendix. On slowly varying averages

In this appendix, we discuss the notion of slow variation of Section 2.2. First, we formulate an example of a condition on $\{\zeta_i^\epsilon\}$ such that respective averages, $\bar{\zeta}_j^\epsilon$, are slowly varying. Further, we study implications for a class of induced averages $\bar{\xi}_j^\epsilon$. The dependence on ϵ will be suppressed.

Take $n_j = n = o(N) \gg 1$ for $j = 1, \dots, M$, i.e., equal number of steps in each I_j. (Recall: $N = Mn$, $M, N \to \infty$). Prescribe a bounded sequence $\{\zeta_i\}_{i=0}^{N-1}$ such that its subsequences within numerous adjacent I_j's are close in the l^1-sense. Specifically, for any $0 < \sigma \ll 1$ there exist positive integers $j_*(M) = o(M)$ and $j_\circ(M)$ with $M - j_\circ = o(M)$ such that, for each $j_* \leq j \leq j_\circ$,

$$\begin{aligned}&\sum_{i\in I_j} |\zeta_{i+k} - \zeta_i| < \sigma \sum_{i\in I_j} |\zeta_i| \quad \text{for all } |k| < k_\circ(\sigma) \\ &\quad \text{if } M > M_\circ(\sigma),\end{aligned} \tag{A.1}$$

where $k_\circ = p_\circ n = o(N)$ and $p_\circ = o(M)$; in particular, $\sigma \downarrow 0$ as $M_\circ, np_\circ \to \infty$. We will refer to such a sequence $\{\zeta_i\}$ as 'admissible'. This construction trivially includes bi-phasic surface reconstructions of Si(001), where $\{\zeta_i\}$ may contain, e.g., alternating diffusivities. We restrict attention to admissible $\{\zeta_i\}$.

Proposition A.1. *Suppose $f : \mathbb{R} \to \mathbb{R}$ is Lipschitz continuous with $f(\zeta) > 0$ for $\zeta \neq 0$; and $\{\zeta_i\}_{i=0}^{N-1}$ is bounded and admissible as $N \to \infty$. In particular, assume that $0 < \alpha \leq |\zeta_i| \leq \beta$ for each i. Define $\bar{\zeta}_j := n^{-1} \sum_{i\in I_j} f(\zeta_i)$. Then, $\bar{\zeta}_j$ are slowly varying.*

Proof. The proof follows directly from Definition 2. First, we note that $\bar{\zeta}_j$ have a fixed, positive greatest lower bound. Let $\bar{\alpha} = \min_j\{\bar{\zeta}_j\}$. Accordingly, we obtain an estimate for the quotient $\delta^p\bar{\zeta}_j$:

$$\begin{aligned}|\delta^p \bar{\zeta}_j| &\leq (pn)^{-1} \sum_{i\in I_j} |f(\zeta_{i+k(p)}) - f(\zeta_i)| \\ &\leq \mathrm{Lip}[f]\,(pn)^{-1} \sum_{i\in I_j} |\zeta_{i+k(p)} - \zeta_i| \\ &\leq C\sigma \left(n^{-1} \sum_{i\in I_j} |\zeta_i|\right) \leq C\sigma, \quad k = np,\end{aligned} \tag{A.2}$$

by virtue of the boundedness of $|\zeta_i|$, provided $j_* \leq j \leq j_\circ$ and $-p_\circ < p < p_\circ$, by the prescription of $\{\zeta_i\}$. Thus, for sufficiently large M, the σ can be made small enough so that $|p\delta^p\bar{\zeta}_j| \ll \bar{\alpha}$ for appropriate j and p. $\square$

Proposition A.2. *Suppose $f : \mathbb{R} \to \mathbb{R}$ is Lipschitz continuous with $f(\zeta) > 0$ for $\zeta \neq 0$; and $\{\zeta_i\}_{i=0}^{N-1}$ and $\{\xi_i\}_{i=0}^{N-1}$ are bounded and admissible. In particular, assume that $0 < \alpha \leq |\zeta_i| \leq \beta$ for each i. Then, the averages $\bar{\xi}_j$ of $\{\xi_i\}$ induced by $\{\zeta_i\}$ via f are slowly varying.*

Proof. Consider Definition 6 for induced averages. Without further ado, we estimate $\delta^p[f(\bar{\zeta}_j)\bar{\xi}_j]$ for $p \neq 0$:

$$
\begin{aligned}
|\delta^p[f(\bar{\zeta}_j)\bar{\xi}_j]| \le{} & (np)^{-1}\sum_{i\in I_j}(|f(\zeta_{i+np})||\xi_{i+np}\xi_i| \\
& + |f(\zeta_{i+np}) - f(\zeta_i)||\xi_i|) \\
\le{} & Cn^{-1}\sum_{i\in I_j}(|\xi_{i+np} - \xi_i| + |\zeta_{i+np} - \zeta_i|) \\
\le{} & C\sigma\, n^{-1}\sum_{i\in I_j}(|\xi_i| + |\zeta_i|) \le C\sigma, \qquad \text{(A.3)}
\end{aligned}
$$

where we used the Lipschitz continuity of f; $\sigma = \max(\sigma_\xi, \sigma_\zeta)$ and σ_ℓ is the constant entering the admissibility definition of $\{\ell_i\}$ for $\ell = \xi,\ \zeta$. By Proposition A.1, the $f(\bar{\zeta}_j)$ is also slowly varying. □

References

[1] J.W. Evans, P.A. Thiel, M.C. Bartelt, Morphological evolution during epitaxial thin film growth: formation of 2D islands and 3D mounds, Surf. Sci. Rep. 61 (2006) 1–128.

[2] H.-C. Jeong, E.D. Williams, Steps on surfaces: experiments and theory, Surf. Sci. Rep. 34 (1999) 171–294.

[3] T. Michely, J. Krug, Islands, Mounds and Atoms: Patterns and Processes in Crystal Growth Far From Equilibrium, Springer-Verlag, 2004.

[4] W.E, N.K. Yip, Continuum theory of epitaxial growth. I, J. Stat. Phys. 104 (2001) 221–253.

[5] D. Margetis, R.V. Kohn, Continuum theory of interacting steps on crystal surfaces in $2 + 1$ dimensions, Multiscale Model. Simul. 5 (2006) 729–758.

[6] P. Nozières, On the motion of steps on a vicinal surface, J. Phys. (France) 48 (1987) 1605–1608.

[7] M. Ozdemir, A. Zangwill, Morphological equilibration of a corrugated crystalline surface, Phys. Rev. B 42 (1990) 5013–5024.

[8] P. Politi, J. Villain, Ehrlich–Schwoebel instability in molecular-beam epitaxy: a minimal model, Phys. Rev. B 54 (1996) 5114–5129.

[9] A. Rettori, J. Villain, Flattening of grooves on a crystal surface: A method of investigation of surface roughness, J. Phys. (France) 49 (1988) 257–267.

[10] O. Pierre-Louis, Step bunching with general step kinetics: stability analysis and macroscopic models, Surf. Sci. 529 (2003) 114–134.

[11] D. Margetis, Homogenization of reconstructed crystal surfaces: Fick's law of diffusion, Phys. Rev. E 79 (2009) 052601.

[12] F. Murat, L. Tartar, On the control of coefficients in PDEs, in: A. Cherkaev, R.V. Kohn (Eds.), Topics in Mathematical Modeling of Composite Materials, in: Progress in Nonlinear PDEs and Their Applications, vol. 31, Birkhäuser, Boston, 1997, pp. 1–8.

[13] L. Tartar, Estimation of homogenized coefficients, in: A. Cherkaev, R.V. Kohn (Eds.), Topics in Mathematical Modeling of Composite Materials, in: Progress in Nonlinear PDEs and Their Applications, vol. 31, Birkhäuser, Boston, 1997, pp. 9–20.

[14] J. Krug, Introduction to step dynamics and step instabilities, in: A. Voigt (Ed.), Multiscale Modeling of Epitaxial Growth, in: International Series of Numerical Mathematics, vol. 149, Birkhäuser, Basel, 2005, pp. 69–95.

[15] C. Misbah, O. Pierre-Louis, Y. Saito, Crystal surfaces in and out of equilibrium: a modern view, Rev. Modern Phys. 82 (2010) 981–1040.

[16] C.B. Duke, Semiconductor surface reconstruction: the structural chemistry of two-dimensional surface compounds, Chem. Rev. 96 (1996) 1237–1260.

[17] V.G. Lifshits, A.A. Saranin, A.V. Zotov, Surface Phases on Silicon: Preparation, Structures and Properties, Wiley, New York, 1994.

[18] W. Mönch, Semiconductor Surfaces and Interfaces, Springer, Berlin, 1995.

[19] G.P. Srivastava, Theory of semiconductor surface reconstruction, Rep. Prog. Phys. 60 (1997) 561–613.

[20] T.J. Stasevich, C. Tao, W.G. Cullen, E.D. Williams, T.L. Einstein, Impurity decoration for crystal shape control: C_{60} on Ag(111), Phys. Rev. Lett. 102 (2009) 085501.

[21] A. Tamai, W. Auwärter, C. Cepek, F. Baumberger, T. Greber, J. Osterwalder, One-dimensional chains of C_{60} molecules on Cu(221), Surf. Sci. 566–568 (2004) 633–637.

[22] P.L. Hansen, J.B. Wagner, S. Helveg, J.-B. Rostrup-Nielsen, B.S. Clausen, H. Topsøe, Atom-resolved imaging of dynamic shape changes in supported copper nanocrystals, Science 295 (2002) 2053–2055.

[23] D.J. Eaglesham, F.C. Unterwald, D.C. Jacobson, Growth morphology and the equilibrium shape: the role of surfactants in Ge/Si island formation, Phys. Rev. Lett. 70 (1993) 966–969.

[24] M. Kalff, G. Comsa, T. Michely, How sensitive is epitaxial growth to adsorbates? Phys. Rev. Lett. 81 (1998) 1255–1258.

[25] G.W. Milton, The Theory of Composites, Cambridge University Press, Cambridge, UK, 2002.

[26] S. Nemat-Nasser, M. Hori, Micromechanics: Overall Properties of Heterogeneous Materials, Elsevier, Amsterdam, 1999.

[27] M.H. Holmes, Introduction to Perturbation Methods, Springer, New York, 1998.

[28] W.K. Burton, N. Cabrera, F.C. Frank, The growth of crystals and the equilibrium structure of their surfaces, Philos. Trans. R. Soc. London Ser. A 243 (1951) 299–358.

[29] O.L. Alerhand, A.N. Berker, J.D. Joannopoulos, D. Vanderbilt, R.J. Hamers, J.E. Demuth, Finite-temperature phase diagram of vicinal Si(100) surfaces, Phys. Rev. Lett. 64 (1990) 2406–2409.

[30] B.S. Swartzentruber, N. Kitamura, M.G. Lagally, M.B. Webb, Behavior of steps on Si(001) as a function of vicinality, Phys. Rev. B 47 (1993) 13432–13441.

[31] V.I. Marchenko, A.Ya. Parshin, Elastic properties of crystal surfaces, Sov. Phys. JETP 52 (1980) 129–131.

[32] D. Margetis, P.-W. Fok, M.J. Aziz, H.A. Stone, Continuum theory of nanostructure decay via a microscale condition, Phys. Rev. Lett. 97 (2006) 096102.

[33] A. Bensoussan, J.L. Lions, G.C. Papanicolaou, Asymptotic Analysis of Periodic Structures, North Holland, Amsterdam, 1978.

[34] G.A. Pavliotis, A.M. Stuart, Multiscale Methods: Averaging and Homogenization, Springer, New York, 2007.

[35] G. Ehrlich, F. Hudda, Atomic view of surface diffusion: Tungsten on tungsten, J. Chem. Phys. 44 (1966) 1039–1099.

[36] R.L. Schwoebel, E.J. Shipsey, Step motion on crystal surfaces, J. Appl. Phys. 37 (1966) 3682–3686.

[37] R. Najafabadi, D.J. Srolovitz, Elastic step interactions on vicinal surfaces of fcc metals, Surf. Sci. 317 (1994) 221–234.

[38] E.E. Gruber, W.W. Mullins, On the theory of anisotropy of crystalline surface tension, J. Phys. Chem. Solids 28 (1967) 875–887.

[39] A. Friedman, Variational Principles and Free-Boundary Problems, Dover, New York, 2010.