

Phase-field model for reconstructed stepped surface

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We formulate a phase-field, or diffuse-interface, model for the evolution of stepped surfaces under surface diffusion in the presence of *distinct* material parameters across nanoscale terraces. In the sharp-interface limit, our model reduces to a Burton-Cabrera-Frank (BCF)-type theory for the motion of noninteracting steps separating inhomogeneous terraces. This setting aims to capture features of reconstructed semiconductor, e.g., Si surfaces below the roughening transition. Our work forms an extension of the phase-field construction by Hu *et al.* [*Physica D* **241**, 77 (2012)].

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I. INTRODUCTION

Surface reconstruction (SR) amounts to the presence of distinct structural phases on certain crystal surfaces, especially those of semiconductors; such phases depend on temperature and misorientation angle [1,2]. For example, many disparate phases on Si surfaces have been observed [3]. A well-known type of SR on Si(100) is manifested by the formation of dimer rows in directions parallel and perpendicular to line defects (steps) below the roughening transition [4–6]. Kinetic rates, e.g., diffusivities and other material parameters then may vary dramatically across neighboring terraces (regions separating steps) whose properties reflect the distinct phases. The mesoscale and macroscale behavior of the surface emerging from such *inhomogeneities* needs to be explored.

Below the roughening transition, the crystal surface morphological evolution is driven by the motion of steps of atomic height a , according to the Burton-Cabrera-Frank (BCF) model [7,8]. Linking step kinetics to the meso- and large-scale surface behavior can contribute to understanding how microscale parameters can be engineered to achieve appealing surface morphologies. This connection is largely unexplored. A partial differential equation (PDE) for the relaxation of the large-scale height profile was formally derived for reconstructed surfaces in one spatial dimension (1D) [9]. However, a systematic, general macroscopic theory is still elusive.

In this Brief Report, we present the formulation of a phase-field model aiming to capture salient features of a reconstructed surface with noninteracting steps in two spatial dimensions (2D). The diffusion of adsorbed atoms (adatoms) and attachment/detachment of atoms at steps, which are key processes of the BCF theory [7], have kinetic rates that *vary* across terraces. Ehrlich-Schwobel (ES) barriers [10], step edge diffusion, desorption, and material deposition from above are included. Our work was inspired by and forms a nontrivial extension of [11]; see also [12–14].

Our motivation is twofold. First, it is broadly known that phase-field models, which replace each step edge by a diffuse boundary layer, are computationally appealing [15]; their use circumvents the need for explicitly tracking steps, which are sharp boundaries in the BCF theory.

Second, the phase-field model provides a natural linkage of microscale (step) motion to the mesoscale *and* macroscale

properties of the surface. The mesoscale comprises the collective behavior of a few atomic steps, at length scales roughly in the range 10–100 nm. This approach should capture heterogeneities not seen by the fully macroscopic description.

The full macroscale theory of reconstructed surfaces should incorporate some notion of averaging over distinct material parameters [9]. Determining such averages in 2D is an open problem. We do not address this issue here, but expect that the phase field model can be explored computationally for further insights in this direction. Numerical computations lie beyond our scope.

The phase field gives rise to a continuum theory since step edges are smoothed out. At the same time, the boundary layer width ϵ controls the influence of boundary conditions at steps. Recovering the sharp-interface limit (BCF-type model) requires $\epsilon \rightarrow 0$.

Our model has limitations. As in [11], step interactions are neglected; the incorporation of force monopole-dipole and other interactions is the subject of work in progress. Furthermore, we neglect anisotropy in terrace diffusion.

The remainder of this Brief Report is organized as follows. Section II revisits elements of the BCF theory and outlines equations of motion for steps. In Sec. III, we formulate the phase-field model, extending related ideas of [11]. In Sec. IV, we argue that the phase-field model yields the BCF-type theory. Lastly, Sec. V summarizes our results and discusses possible implications.

II. ELEMENTS OF BCF-TYPE THEORY

We start with elements of step motion [7]. The kinetic processes are: (i) diffusion of adatoms on terraces and step edges; (ii) attachment and detachment of atoms at steps; (iii) desorption; and (iv) material deposition from above. Our model uses distinct diffusivities (on terraces and step edges) and sticking rates for atoms at steps.

First, we outline the step geometry. Consider N monolayers (or ordered steps); see Fig. 1. Let \mathcal{U}_i and Γ_i denote the i th terrace and step edge, respectively, where each Γ_i is smooth and non-self-intersecting; for steps, $i = 1, \dots, N$, $N \gg 1$, and Γ_0 lies far away from Γ_N .

Adatom diffusion is characterized by the (positive) diffusivity D_i in each region \mathcal{U}_i ; in addition, atoms attach/detach

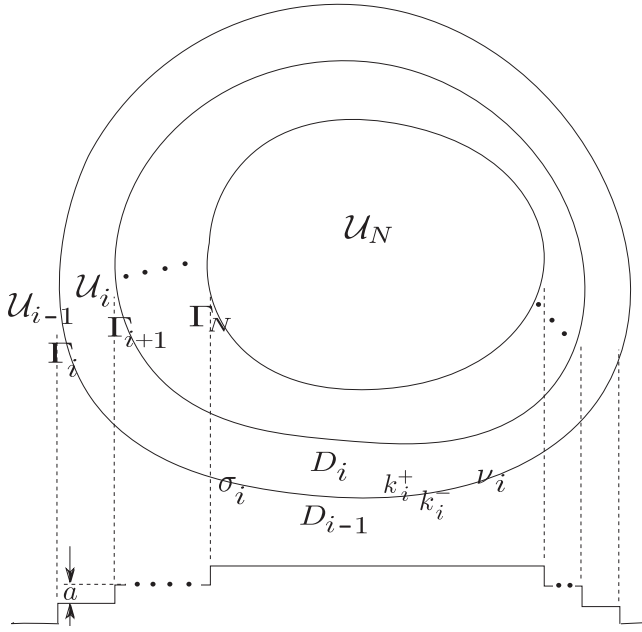


FIG. 1. Top and side views of steps and terraces in 2D. \mathcal{U}_i denotes the i th terrace ($i = 0, \dots, N$), and Γ_i denotes the i th step edge ($i = 1, \dots, N$). The parameters σ_i , k_i^\pm , and ν_i/a denote step stiffness, attachment/detachment rates, and step-edge diffusivity on Γ_i ; and D_i is the adatom diffusivity on \mathcal{U}_i . The step height is a constant, a .

with kinetic rates k_i^\pm at Γ_i from the upper (+) or lower (−) terrace; see Eqs. (1) below. An example of a system with such terrace-dependent diffusivities is the reconstructed Si(111) which exhibits two phases simultaneously, with two values of D_i periodically alternating from one terrace to the next [3].

Now define $C_i = C_i(x, y, t)$ and $\mathbf{J}_i = -D_i \nabla C_i$ as the adatom density and flux on the i th terrace of the (x, y) -plane (basal plane). The adatom concentration satisfies $\partial_t C_i + \nabla \cdot \mathbf{J}_i = \mathcal{F} - \tau^{-1} C_i$ in \mathcal{U}_i , where \mathcal{F} is the deposition flux and τ is the desorption time. We employ the quasisteady approximation, $\partial_t C_i \simeq 0$ for small enough \mathcal{F} , by which $\nabla \cdot \mathbf{J}_i \simeq \mathcal{F} - \tau^{-1} C_i$. Further, we apply linear kinetics for atom attachment/detachment at steps:

$$\mathbf{J}_i \cdot \mathbf{n}_i = k_i^+ (C_i - C_i^{\text{eq}}) \quad \text{on } \Gamma_i, \quad (1a)$$

$$-\mathbf{J}_{i-1} \cdot \mathbf{n}_i = k_i^- (C_i - C_i^{\text{eq}}) \quad \text{on } \Gamma_i, \quad (1b)$$

where \mathbf{n}_i is the in-plane unit vector normal to Γ_i pointing outward from \mathcal{U}_i , and k_i^+ (k_i^-) is the adatom attachment-detachment rate from the upper (lower) terrace at the i th step edge; for a positive ES barrier [10], we assume $k_i^+ < k_i^-$. If steps do not interact, the equilibrium concentration C_i^{eq} is given by [8]

$$C_i^{\text{eq}} \simeq C_* (1 + \sigma_i \kappa_i), \quad (2)$$

where C_* and σ_i are constants and κ_i is the (local) curvature of Γ_i ; $\sigma_i = \zeta_i / (k_B T)$, ζ_i is the i th step stiffness, and $k_B T$ is the Boltzmann energy (absolute temperature).

A few remarks on the omitted step-step interactions are in order. It is known that surface reconstruction can generate internal stresses, because of which steps can exhibit force monopole-dipole interactions [6,16]. These interactions

modify Eq. (2) to $C_i^{\text{eq}} \simeq C_* (1 + \sigma_i \kappa_i + e_i)$, where the interaction term e_i may have tractable forms in relatively simple, e.g., radial step geometries in 2D. Thus far, we have been unable to formulate a phase-field model with a nonzero e_i .

The diffusion equation for C_i along with Eqs. (1) and (2) are complemented with the step velocity law, $v_i = (\Omega/a)(\mathbf{J}_i - \mathbf{J}_{i-1}) \cdot \mathbf{n}_i + a \partial_{s_i} (v_i \partial_{s_i} \kappa_i)$ on Γ_i , where v_i is the normal velocity of the i th step edge, $\Omega \simeq a^3$ is the atomic volume, and ∂_{s_i} is the partial derivative with respect to the step-edge arc length s_i . The last term in the equation for the step velocity describes step-edge diffusion with coefficient $v_i a^{-1}$; by this effect, atoms are most inclined to attach to points with a relatively high rate of change in curvature [17]. We assume that $\Gamma_0 \equiv \Gamma_\infty$ is a large circle of radius R_∞ , a typical macroscopic length. By a uniform-far-field condition [11], we require that $\frac{1}{2\pi} \int_{\Gamma_\infty} \mathbf{J}_0 \cdot \mathbf{n}_0 dS = J_\infty$, and set $J_\infty = 0$ for later algebraic convenience.

Next, we nondimensionalize time and spatial variables by introducing $t_* = R_\infty^2 / D$ and $\ell_* = R_\infty$; D is a reference value for the diffusivities, say, $D = D_0$. Set $\tilde{t} = t/t_*$ and $(\tilde{x}, \tilde{y}) = (x/\ell_*, y/\ell_*)$, $\tilde{a} = a/\ell_*$. Define the nondimensional concentration and flux: $\varrho_i = \ell_*^2 (C_i - C_*)$ and $\mathcal{J}_i = -\mathcal{D}_i \tilde{\nabla} \varrho_i$, where $\mathcal{D}_i = D_i/D$ and $\tilde{\nabla} = (\partial_{\tilde{x}}, \partial_{\tilde{y}})$. The adatom diffusion equation and step velocity law read

$$\tilde{\nabla} \cdot \mathcal{J}_i = \Lambda - \zeta^2 (\varrho_i + \varrho_*) \quad \text{in } \mathcal{U}_i, \quad (3)$$

$$\tilde{v}_i \tilde{a}^{-2} = (\mathcal{J}_i - \mathcal{J}_{i-1}) \cdot \mathbf{n}_i + \tilde{a}^{-1} \partial_{\tilde{s}_i} (\beta_i \tilde{\partial}_{\tilde{s}_i} \tilde{\kappa}_i) \quad \text{on } \Gamma_i, \quad (4)$$

where the tildes express the scaled-coordinate system. The kinetic boundary conditions at step edges read

$$\xi_i^+ \mathcal{J}_i \cdot \mathbf{n}_i = \varrho_i - \varrho_* \delta_i \tilde{\kappa}_i \quad \text{on } \Gamma_i, \quad (5a)$$

$$-\xi_i^- \mathcal{J}_{i-1} \cdot \mathbf{n}_i = \varrho_{i-1} - \varrho_* \delta_i \tilde{\kappa}_i \quad \text{on } \Gamma_i. \quad (5b)$$

In Eqs. (3)–(5), $\tilde{v}_i = (\ell_*/D)v_i$, $\Lambda = \mathcal{F} \ell_*^4 / D$, $\zeta = \ell_*/\sqrt{D\tau}$, $\xi_i^\pm = D/(k_i^\pm \ell_*)$, $\delta_i = \sigma_i / \ell_*$, $\tilde{\kappa}_i = \ell_* \kappa_i$, $\varrho_* = C_* \ell_*^2$, and $\beta_i = v_i / (\ell_* D)$. For ease of notation, we henceforth drop the tildes.

III. PHASE-FIELD MODEL

We now focus on the phase-field variable (order parameter) $\phi^\epsilon(x, y, t)$, a smooth approximation for the (discrete) height of the step configuration [11]; $\phi^\epsilon = ia$ on the i th terrace. Our goal is to replace the BCF-type model of Eqs. (3)–(5) by evolution laws involving ϕ^ϵ . These laws account for: (i) the rapid change of ϕ^ϵ across boundary layers (narrow regions near steps), and (ii) the condition that ϕ^ϵ approaches its appropriate constant value on each terrace away from steps. These two distinct behaviors are matched to produce a solution everywhere.

Our model contains the step-number-dependent material parameters ξ_i^\pm , \mathcal{D}_i , δ_i , and β_i ; in contrast, in [11] each of these parameters is constant. This feature is reflected into the respective evolution laws for ϕ^ϵ , Eqs. (6) and (7).

Equation (3) is replaced by the evolution law

$$\begin{aligned} a^{-2} [a^{-1} \partial_t \phi^\epsilon - \nabla_s \cdot (\beta \nabla_s \kappa)] \nabla \phi^\epsilon & \\ = \nabla \cdot [M(\phi^\epsilon; \epsilon) \nabla \varrho^\epsilon] + \Lambda - \zeta^2 (\varrho^\epsilon + \varrho_*), & \quad (6) \end{aligned}$$

where $\varrho^\epsilon(x, y, t)$ is a field variable that smoothly approximates the adatom density, ϱ_i ; $\kappa = \nabla \cdot \mathbf{n}^\epsilon$ and $\mathbf{n}^\epsilon = -\nabla \phi^\epsilon / |\nabla \phi^\epsilon|$ define the local curvature of and unit vector normal to level

sets of ϕ^ϵ , i.e., (x, y) -curves on which $\phi^\epsilon = \text{const.}$, respectively [18]. Also, $\nabla_s = (\mathbf{I} - \mathbf{n}^\epsilon \mathbf{n}^\epsilon) \nabla$ (\mathbf{I} : unit tensor) is the gradient along ϕ^ϵ -level sets. Step velocity law (4) and conditions (5) are replaced by

$$\begin{aligned} & \alpha a^{-2} \epsilon^2 [a^{-1} \partial_t \phi^\epsilon - \nabla_s \cdot (\beta \nabla_s \kappa) |\nabla \phi^\epsilon|] \\ & = \epsilon^2 \Delta \phi^\epsilon - G'(\phi^\epsilon) + \frac{\epsilon \vartheta}{\varrho_*} \varrho^\epsilon, \end{aligned} \quad (7)$$

where the prime denotes differentiation with respect to the argument. The coefficients of Eqs. (6) and (7) are defined below. These equations are supplemented with the boundary conditions that the normal derivatives of ϕ^ϵ and ϱ^ϵ vanish at Γ_∞ . Unlike the description in [13], Eqs. (6) and (7) do not contain a time derivative of ϱ^ϵ because of the quasisteady approach. In the limit $\epsilon \rightarrow 0$, Eq. (6) reduces to Eq. (3) on each terrace, and both Eqs. (6) and (7) contribute to Eqs. (4) and (5) at steps.

We further comment on Eqs. (6) and (7). *The continuous mobility M accounts for inhomogeneities due to ξ_i^\pm and \mathcal{D}_i :* $M(\phi; \epsilon) = \mathfrak{M}(\phi) [1 + \epsilon^{-1} \zeta(\phi)]^{-1}$. Here, \mathfrak{M} is a smooth function for terrace (i)-dependent diffusivities,

$$\mathfrak{M}(\phi) = \eta_{a/4}(\phi) * \sum_i \mathcal{D}_i \chi_{[(i-1/2)a, (i+1/2)a)}(\phi),$$

where $\eta_{a/4}(\phi) = \frac{4}{a} \eta(\frac{4\phi}{a})$ is a mollifier with, e.g., $\eta(x) = C \exp[1/(|x|^2 - 1)]$ if $|x| < 1$ and 0 if $|x| \geq 1$ so that $\int_{-\infty}^{\infty} \eta(x) dx = 1$; the $*$ operation denotes convolution; and $\chi_S(\phi) = 1$ if ϕ lies in set S and 0 otherwise. Step-dependent sticking rates are included in $\zeta(\phi) = \gamma_i [\phi - (i-1)a]^{p_i} (ia - \phi)^{q_i} G(\phi)$ for $\phi \in [(i-1)a, ia]$ [19], where γ_i , p_i , and q_i satisfy

$$\alpha = \frac{1}{\varrho_* \delta} \int_0^a \frac{\zeta(\phi + (i-1)a)}{\mathfrak{M}(\phi + (i-1)a) \sqrt{2G(\phi)}} \phi(a - \phi) d\phi, \quad (8)$$

$$\xi_i^- = \int_0^a \frac{\zeta(\phi + (i-1)a)}{\mathfrak{M}(\phi + (i-1)a) \sqrt{2G(\phi)}} (a - \phi) d\phi, \quad (9)$$

$$\xi_i^+ = \int_0^a \frac{\zeta(\phi + (i-1)a)}{\mathfrak{M}(\phi + (i-1)a) \sqrt{2G(\phi)}} \phi d\phi. \quad (10)$$

The function $G(\phi)$ is the periodic multiwell free energy $G(\phi) = [e^{f_i(\phi)} - 1][e^{f_{i+1}(\phi)} - 1]$ for $\phi \in [ia, (i+1)a]$ [11, 13]; $f_i(\phi) = c_1(ia - \phi)^2 + c_2(ia - \phi)^4$ where c_1 and c_2 are constants chosen conveniently for applications; for example, take $c_1 = 4.5$ and $c_2 = 0.9$ in [11]. Note that G changes rapidly away from step edges and indicates the position of terraces as a function of the height profile. For each i , the function $\vartheta(\phi)$ is defined on $[(i-1)a, ia]$ by $\vartheta(\phi) = K_i [\varpi(\phi) \int_{(i-1/2)a}^\phi G(w)^{-1} dw]^{-1}$ for $\phi \neq (i-1)a, ia$ and 0 for $\phi = (i-1)a, ia$, where $\varpi(\phi) = -1$ if $\phi < (i-1/2)a$ and 1 otherwise, and the constant K_i is chosen so that $\delta_i = \int_{(i-1)a}^{ia} \vartheta(\phi)^{-1} \sqrt{2G(\phi)} d\phi$.

In Eqs. (6) and (7) we invoke the continuous function $\beta(\phi; \epsilon) = \sum_i (\beta_i - \beta_{i-1}) \{1 + e^{-\frac{[\phi - (i-1)a]}{\epsilon}}\}^{-1}$ which accounts for step edge diffusion, with $\beta_0 \equiv 0$. The constant l is positive and determines how fast β converges (as $\epsilon \rightarrow 0$) to the discontinuous function $\sum_{i=1}^N \beta_i \chi_{[(i-1)a, ia)}(\phi)$; for all practical purposes, set $l = 1$.

Our definition of the mobility function $M(\phi; \epsilon)$ differs from the corresponding formulation in [11] where $\mathfrak{M}(\phi)$ is unity and the coefficients of $\zeta(\phi)$ do not depend on i . In particular, our $M(\phi; \epsilon)$ is nonperiodic so that it can accommodate distinct diffusivities (whereas M is periodic in [11]). Note that $\mathfrak{M}(\phi) \equiv \mathcal{D}_i$ if ϕ lies in $[(i - \frac{1}{4})a, (i + \frac{1}{4})a]$. In Sec. IV, we indicate how this \mathfrak{M} leads to the terrace-dependent Eq. (3). Also, we introduce i -dependent parameters p_i , γ_i , and q_i in $\zeta(\phi)$ to compensate for the i dependence of ξ_i^\pm and the lack of periodicity of $M(\phi)$. Physically, this ζ yields the asymmetry of the ES barrier.

In view of the above, the BCF-type limit is described via ϕ^ϵ . By defining $\Gamma_i(t; \epsilon)$ so that $\phi^\epsilon(x, y, t) = (i - 1/2)a$ for (x, y) in $\Gamma_i(t; \epsilon)$, the sharp interface stems from the limit $\Gamma_i(t; 0) \equiv \Gamma_i$ of $\Gamma_i(t; \epsilon)$ as $\epsilon \rightarrow 0$. In this limit, $\mathbf{n}^\epsilon \rightarrow \mathbf{n}|_{\epsilon=0}$, which is the unit vector normal to step edges in the (x, y) -plane [18].

IV. DISCUSSION: ASYMPTOTIC MATCHING

Following [11], we briefly discuss how our phase-field model yields the BCF-type model. The idea is to separate the spatial coordinate normal to each step into fast (z_i) and slow (r_i) variables. In the inner regions (boundary layers), the variation of ϕ^ϵ over z_i prevails; and in the outer regions the slow variable is important. A global solution for ϕ^ϵ is obtained by appropriate matching.

To describe ϕ^ϵ near the i th step, consider the orthogonal curvilinear coordinate system (r_i, s_i) near $\Gamma_i(t; \epsilon)$; $r_i = r_i^\epsilon(x, y, t)$ is the signed distance of (x, y) from $\Gamma_i(t; \epsilon)$ where $r_i > 0$ in the direction of \mathcal{U}_{i-1} , and $s_i = s_i^\epsilon(x, y, t)$ is the arc length along $\Gamma_i(t; \epsilon)$ [11]. By $z_i = r_i/\epsilon$, define $\Phi(z_i, s_i, t; \epsilon) = \phi^\epsilon(x, y, t)$ and $P(z_i, s_i, t; \epsilon) = \hat{Q}^\epsilon(r_i, s_i, t) = \varrho^\epsilon(x, y, t)$ in the inner region. We make explicit the dependence on ϵ of each relevant variable (Q) by expanding $Q = Q^{(0)} + \epsilon Q^{(1)} + \epsilon^2 Q^{(2)} + \dots$ (e.g., $Q = \Phi$) [11].

Our model uses continuous functions such as $\mathfrak{M}(\phi)$ to reconcile the distinct microscale parameters, e.g., \mathcal{D}_i with the smooth transition of the phase field ϕ^ϵ from each boundary layer to the outer region. Across the boundary layer, the terrace diffusion function \mathfrak{M} , a constant in [11], varies from one diffusivity to another. Since \mathfrak{M} is independent of ϵ , this transition is smooth even in the limit $\epsilon \rightarrow 0$ and does not affect the resulting diffusion equation on terraces. The edge diffusion function $\beta(\phi)$ remains a constant (β_i) in the i th boundary layer and varies smoothly from β_i to β_{i+1} on the i th terrace. However, this behavior does not alter Eq. (3) because β is multiplied by $|\nabla \phi^\epsilon|$ which vanishes on terraces to leading order in ϵ . The smooth function $\zeta(\phi)$ is properly integrated over the boundary layer to yield the distinct sticking rates ξ_i^\pm . Note that ζ has no effect on any terrace because $\zeta(ia) = 0$ for all i . Also, $\vartheta(\phi)$ does not appear in the leading outer expansion; the magnitude of ϑ (determined by K_i) accommodates an i -dependent stiffness.

By skipping details, we now indicate the sharp-interface limit. In the outer region, Eq. (7) yields $G'(\phi^{(0)}) = 0$ to leading order in ϵ ; thus, $\phi^{(0)} = (i-1)a, ia$. This implies that as $\epsilon \rightarrow 0$, $\Gamma_i(t; 0) \equiv \Gamma_i$ lies between two terraces of heights $(i-1)a$ and ia . Thus, we find $\zeta(\phi^{(0)}) = 0$ and $M(\phi^{(0)}; \epsilon) = \mathcal{D}_i$ on the i th terrace. Hence, Eq. (6) produces Eq. (3) to leading order.

In the overlap region near each terrace, every ϕ^ϵ -dependent quantity from the outer region must coincide with the limit of the respective variable from the inner region. For example, as (x, y) approaches Γ_i , $\phi^{(0)}$ from the outer region tends to the limit of $\Phi^{(0)}(z_i, s_i, t)$ as $z_i \rightarrow \pm\infty$; thus, the matching gives $\lim_{z_i \rightarrow -\infty} \Phi^{(0)} = ia$ [11]. Such conditions are incorporated in the inner region as boundary conditions to the appropriate expansions in ϵ of Eqs. (6) and (7) to obtain Eqs. (4) and (5).

V. CONCLUSION

We presented a phase-field model for the near-equilibrium evolution of stepped surfaces with distinct inhomogeneities at the microscale. This work forms an extension of the formulation in [11]. A particular feature of our model, absent from [11], is the mobility function $M(\phi^\epsilon; \epsilon)$ that describes sequences of disparate diffusivities D_i and sticking kinetic rates k_i^\pm across terraces and steps. Our analysis also

accounts for arc-length-varying, terrace-dependent step-edge diffusivities.

Our model has limitations, pointing to open questions. We considered noninteracting steps; the incorporation of entropic and other step-step interactions is a pending issue. The numerical simulation of ϕ^ϵ , although appealing for applications, was not touched upon. Similarly, we have not studied possible instabilities that may result in the presence of terrace inhomogeneities; for example, we expect that simulations of the phase-field model can reveal meandering instabilities in the spirit of [20]. The full continuum limit, where $a \rightarrow 0$ and $\epsilon \rightarrow 0$, was not studied; a question is how to implement a reasonable ordering of these limits or scaling of a with ϵ . This task is left for near-future work.

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