Two-dimensional facet nucleation and growth on Si(111)

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The lateral growth of an isolated nucleated facet is studied using a simple two-dimensional step model. An effective Hamiltonian that causes a planar surface to phase separate into facets and step bunches is proposed. The motions of the steps are determined by the relaxational dynamics of the effective Hamiltonian with and without a local conservation requirement. An even simpler mean-field-like model is used to illustrate the mechanism of the experimentally observed constant-velocity facet tip propagation. Numerical calculations using thermodynamic and transport coefficients previously measured give good agreement with experiments under the local conservation requirement. [S0163-1829(97)02808-7]

I. INTRODUCTION

Thermodynamics predicts that a vicinal surface with a single orientation can spontaneously facet into surfaces of different orientations due to an anisotropy in the surface free energy.[1,2] This often occurs when surface adsorption or reconstruction processes stabilize certain preferred orientations. Recently the equilibrium properties of faceted surfaces have been measured with sufficient accuracy that detailed thermodynamic analyses can be carried out.[3–13] Moreover, advances in real-time direct imaging techniques now allow for a detailed description of microscopic kinetic processes.[14,15] Specifically, it has been observed that under certain conditions facets nucleate randomly. They grow at a constant rate along the step direction but grow much more slowly normal to the steps, thus taking on an elongated cigarlike shape.[16] In the case of Si(111), while the thermodynamics of this process is well understood,[11,12,16,17] a complete description of the kinetics has yet to be formulated.

The kinetics of the faceting problem is a subject of long standing in the field of surface science. Mullins[18] proposed a continuum model for facet growth during thermal etching. In this pioneering work, it was shown that the specific kinetic mechanism for mass transport is important in explaining the time evolution of the facet. Mullins assumed that the advancing facet tip would attain a constant steady-state velocity along the step direction. He then calculated the normal surface profile and the characteristic normal growth rate using a one-dimensional model. He found that the normal width of the facet grows as $t^{1/2}$ under an evaporation-condensation mechanism and as $t^{1/4}$ under surface diffusion. While the assumption of steady-state tip propagation has been confirmed by several experimental measurements, the effect of

specific kinetic mechanisms on the growth law for the facet width remains obscure.[16,19]

Mullins's isotropic continuum model does not properly describe the free energy of a surface below the roughening temperature. A one-dimensional step model appropriate for such a surface has been developed by several authors[20–22] and used to explain various interaction-driven phenomena.[23,24] In this paper we extend these ideas and develop a *two-dimensional* step model that can take into account both the step interactions and step meanderings. By introducing some appropriate effective interactions that comply with the thermodynamics of the faceting problem, we can reproduce the steady facet growth along the step direction, and establish the effects of kinetics on the growth of the facet width. We find a relation between the facet growth problem and the general class of reaction-diffusion pattern formation systems.[25] We use as a test example the propaga-
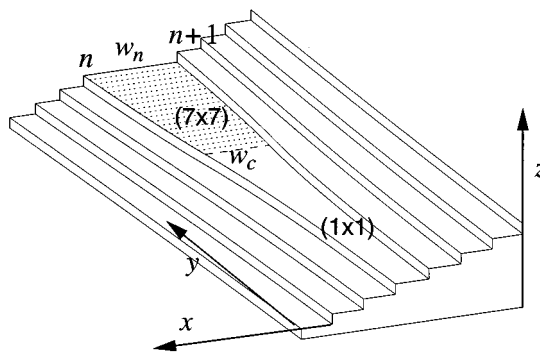

FIG. 1. A schematic picture of the two-dimensional model for the faceting problem.

tion of (7×7) reconstructed facets on Si(111) where the model's parameters have been previously measured.

II. THERMODYNAMICS AND KINETICS OF THE RECONSTRUCTION

The thermodynamics of vicinal Si(111) surfaces near the (7×7) reconstruction transition temperature has been extensively studied.[26] In this section we use a two-dimensional step model as a mesoscopic description of the surface configurations (see Fig. 1).[27] The system consists of a number of steps with the same sign (all ascending or descending). The position of the ith step is denoted by $x_i(y)$, where the y axis coincides with the average orientation of the steps. The y argument is made continuous by coarse graining the system along the step edge direction to a scale large compared to atomic spacing but small compared to typical step patterns of interest. We also assume initially that the step orientation remains predominately along the y direction. We postulate that the effective Hamiltonian of such a coarse-grained system can be written as

$$H = \int dy \sum_i \left[V(w_i(y)) + \frac{\widetilde{\beta}}{2} \left(\frac{\partial x_i(y)}{\partial y} \right)^2 \right] + H_0, \quad (1)$$

where we define the local terrace width $w_i(y) \equiv x_{i+1}(y) - x_i(y)$ for each terrace and y position. Here $\widetilde{\beta}$ is the ''bare'' line tension or step edge stiffness that controls the extent of fluctuations of an *isolated* step in the y direction, while $V(w)$ describes the effective step-step interactions, taken here to be between adjacent steps only. In Eq. (1) we have evaluated the interaction terms at the same y position and linearized the line tension term.[28] When steps are reasonably straight, these should be good approximations, but we will use Eq. (1) even in more general cases as a model. For the present application of the model, steps remain remarkably straight. The angles of the steps with respect to their average orientation are generally less than 3° in the numerical calculations we have carried out.

Next we will try to find the appropriate form for the effective interaction term $V(w)$ for the faceting problem. This should take into account the effects of reconstruction as well as direct elastic or entropic interactions between steps. In one-dimensional models a standard approximation[21,22] sets $V(w) = f(1/w)w$. Here $f(s)$ is the free energy density of a uniform surface with step density $s = 1/w$, projected on a reference (low-index) plane on which the faceting can occur. This procedure associates the free energy *locally* with each terrace, even in cases where neighboring terrace widths vary. The pairwise potential $V(w)$ includes the effects of entropic repulsions between steps that arise physically from step meanderings at different y positions. The essence of this approximation is to average over the effects of these fluctuations by coarse graining the step along the y direction and to study a deterministic process, which in this paper is the growth rate of a facet after it is nucleated. This approach has been implicitly used by Nozières[21] in a one-dimensional dynamical model and subsequently adopted by many authors and compared with experiments recently.[22–24] We assume
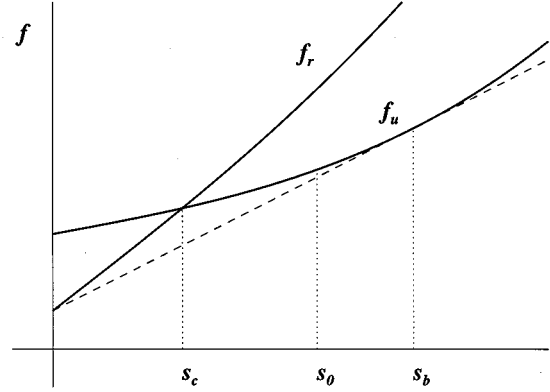

FIG. 2. Illustration of the coarse-grained free energy f as a function of the step density s. The dashed line between s_a and s_b is the tie-bar construction and corresponds to the thermodynamic free energy. The intersection of the two curves gives the critical width for the step model. A proper coarse-grained free energy should round off the cusp but the nucleation growth rate is insensitive to the detailed form of the free energy as long as it gives the correct critical size and energy barrier.

here that our coarse-graining scale in the y direction is large enough that we can use the same functional form for V in our two-dimensional model.[29]

The terrace-step-kink (TSK) model predicts that the variation of surface energy with step density s takes the form[30,31]

$$f_{r,u}(s) = f_{r,u}^0 + \beta_{r,u} s + g_{r,u} h^3 s^3 \quad (2)$$

for vicinal surface, where f^0 is the surface free energy density of the reference plane, β is the free energy cost per unit length of creating an isolated step, h is the step height, and $gh^3 s^3$ is the free energy due to step interactions. Both entropic and elastic interactions can contribute to the last term. The step height h is introduced in Eq. (2) so that the definitions of β and g are the same as in Refs. 11, 12, and 26. The subscripts u and r indicate the values of parameters for systems either completely unreconstructed (u) or reconstructed (r). Reconstruction-induced faceting can be understood by assuming that $f_r^0 < f_u^0$ but that $\beta_r > \beta_u$: while reconstruction lowers the free energy of the reference (flat) surface there is a higher cost associated with the ''broken bonds'' at a step. Thus reconstruction is favored only on sufficiently wide terraces. Figure 2 is an illustration of the free energy curves from Eq. (2) for Si(111) below the transition temperature. For a given step density s only one phase is metastable, corresponding to the lower branch of the two free energy curves. Thermodynamics predicts that eventually the system will ''phase separate,'' with reconstructed flat facets coexisting with unreconstructed step bunches with a step density s_b determined by the familiar tie-bar construction.[11,12]

However, to study the initial dynamics of phase separation, we should use the metastable free energies rather than the limiting thermodynamic ones. Although the detailed shape of the proper free energy functional arising from coarse graining of the microscopic model is important in the study of the initial nucleation event and in a possible spinodal decomposition regime,[32] here we concentrate on the

simpler process of determining the growth rate of an isolated facet after it has nucleated. This permits the use of a simple two-phase model describing the reconstruction of different parts of each terrace.[33] Because of the coarse graining, each terrace is effectively divided up into segments along the y direction. We assume each segment will reconstruct provided its width is larger than some critical width w_c, here determined by the intersection of the two metastable free energy curves in Fig. 2. Hence we assume the effective interaction between steps has the simple form $V(w) = \min\{f_{r,u}(1/w)w\}$. More accurate expressions, incorporating, e.g., preferences for integer multiples of the (7×7) reconstruction unit, could easily be used, but this form seems sufficient for this initial exploration.

The problem of step motions for systems out of equilibrium is generally discussed in the framework of the classical Burton-Cabrera-Frank (BCF) model[34] and its generalizations.[35,36] Although the BCF model is very successful and well grounded physically for the crystal growth problem, its application to a two-dimensional problem is very difficult, requiring the solution of a diffusion equation with moving boundary conditions on arbitrarily shaped step configurations. Also the generalized BCF model involves some physical parameters that are very difficult to measure and introduces the possibility of instabilities such as the Mullins-Sekerka[36] instability which do not seem to be important in the faceting problem. In this paper we discuss two phenomenological approximations that incorporate what we believe to be the essential physics in a simpler way. These can be used for numerical calculations and compared with experiments quantitatively.

The step positions $x_i(y)$ can change due to attachments and detachments of atoms at the step edges. In the coarse-grained model, each atomic attachment/detachment event corresponds to a small variation of the step profile. Therefore the free energy change is proportional to the functional derivative of the effective Hamiltonian. We can define the step edge chemical potential — the change in free energy per atom for adding atoms to the step at coarse-grained position y — as

$$\mu_i(y) = -\Omega \frac{\delta H}{\delta x_i(y)}$$

$$= \Omega[V'(w_i) - V'(w_{i-1}) + \widetilde{\beta}\partial^2 x_i/\partial y^2] + \mu_C, \quad (3)$$

where Ω is the area of the unit cell (the area occupied by an atom at the step edge) and $V'(w)$ is the derivative of $V(w)$ with respect to w. Here μ_C is the atom chemical potential of the solid. In the case of no exchange of atoms between the vapor and solid phase, it is just a Legendre constant chosen to fix the total number of atoms. For simplicity, we neglect the exchange of atoms between the solid and vapor phase, as is the case for Si(111) near the transition temperature from (1×1) to (7×7) reconstruction (850 °C).

In the first approximation, we adopt the idea of the BCF model and assume there is no direct hopping of adatoms between different terraces. We also assume that the main microscopic mechanism for step motion is the exchange of atoms at step edges with adatoms or vacancies on terraces (attachment/detachment processes), which is one possible in-
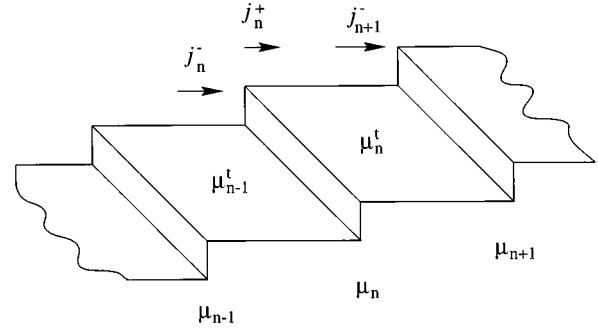

FIG. 3. Illustration of the dynamics of the step motion. At any given y position, we define atomic chemical potential at step edges μ_n and terraces μ_n^t. The flux due to the exchange of atoms between steps and neighboring terraces is determined by the difference of the chemical potentials.

terpretation of the step fluctuations on Si(111) around 900 °C.[37] Then using first order kinetics we can write the flow of atoms from step n to terrace n as (see Fig. 3 for illustration of the labeling)

$$j_n^+(y) = \alpha^+[\mu_n(y) - \mu_n^t(y)], \quad (4)$$

and similarly the flow of atoms from step n to terrace $n-1$ as

$$-j_n^-(y) = \alpha^-[\mu_n(y) - \mu_{n-1}^t(y)], \quad (5)$$

where $\mu_n^t(y)$ is the adatom chemical potential on terrace n at y position. From microscopic mass conservation, the step velocity is

$$\partial x_n(y)/\partial t = \Omega[j_n^+(y) - j_n^-(y)] \quad (6)$$

for small step velocities and low adatom concentrations. We neglect here the gradient of $\mu_n^t(y)$ on the same terrace perpendicular to the step direction by assuming slow attachment/detachment rates and fast diffusion rates, but $\mu_n^t(y)$ can still be different for different terraces and y positions. For simplicity, we assume here symmetric kinetics $(\alpha^+ = \alpha^- = \alpha)$.

Under the quasistatic approximation in the BCF model, at any given time the adatom concentration field satisfies the static diffusion equation. In the limit of no evaporation or deposition, this requires $j_n^+(y) = j_{n+1}^-(y)$, if we neglect the diffusion of adatom along the step direction. Hence we can determine the adatom chemical potential on each terrace by $\mu_n^t(y) = [\mu_n(y) + \mu_{n+1}(y)]/2$ through Eqs. (4) and (5). Thus the equation of motion from Eq. (6) is

$$\frac{\partial x_n(y)}{\partial t} = \frac{\alpha\Omega}{2}[2\mu_n(y) - \mu_{n-1}(y) - \mu_{n+1}(y)]. \quad (7)$$

We call this kinetics with *local conservation of atoms*, because in this case, the motion of each step will affect the motion of neighboring steps not only through energetic interactions, but also from the requirement of conserving atoms on each terrace. We can also obtain some more compli-

cated equations by solving the one-dimensional diffusion equation under general conditions but the essential features are the same.

Strictly speaking, the omission of the adatom diffusion along the step direction can be readily assumed only in the one-dimensional model and is problematic if the diffusion rate along the step direction is very large or the variation of surface profile along the step direction is very large. The local conservation requirement $j_n^+(y) = j_{n+1}^-(y)$ can be further called into question if we allow direct adatom hopping between different terraces. These are the motivations for us to consider a different limit. We now assume there exist some channels for long distance mass movement without the requirement of strict local conservation. The adatoms exchange with a reservoir and act much like a two-dimensional gas. As a result, the adatom chemical potential is the *same* for all the terraces and y positions instead of being determined by the neighboring steps. It is an easy matter to write down the equations of motion for this *nonlocally conserved* case:

$$\frac{\partial x_n(y)}{\partial t} = 2\alpha\Omega[\mu_n(y) - \mu_C]. \tag{8}$$

Equations (7) and (8) are analogous to the equations of motion in Mullins's original paper[18] for the surface diffusion mechanism, and the evaporation-condensation mechanism, respectively. It is easy to implement the two equations of motion numerically and study the evolution of the step configurations. This work is described in Sec. IV.

III. MEAN-FIELD-LIKE MODEL AND STEADY-STATE FRONT PROPAGATION

The model discussed above involves the coupled motion of many meandering steps and the resulting dynamics is quite complicated. Before discussing the numerical calculations and the results of this many-step model, we first study a much simpler model that corresponds to a well understood mathematical problem, where analytical results can be obtained. We assume that reconstruction only occurs on a single terrace and denote the facet width at different y positions by $w(y,t)$. Using a mean-field picture, we assume that the effects of the neighboring steps on the time evolution of the facet width can be approximated by some appropriately chosen *driving force* term $\varphi(w)$ that is a function of the facet width w only. We particularly want to examine the motion of the facet tip. Our model equation for facet motion takes the form

$$\frac{\partial w(y)}{\partial t} = \gamma\frac{\partial^2 w(y)}{\partial y^2} + \varphi(w). \tag{9}$$

The first term on the right describes the step stiffness, which favors straight steps, and the second term qualitatively describes the effect of step interactions and surface reconstruction. This is basically the deterministic part of a Langevin equation for the motion of the steps immediately bounding the facet under the approximation that the influence of more distant steps is described by some effective driving force term $\varphi(w)$ which is a function *only* of the facet width w.
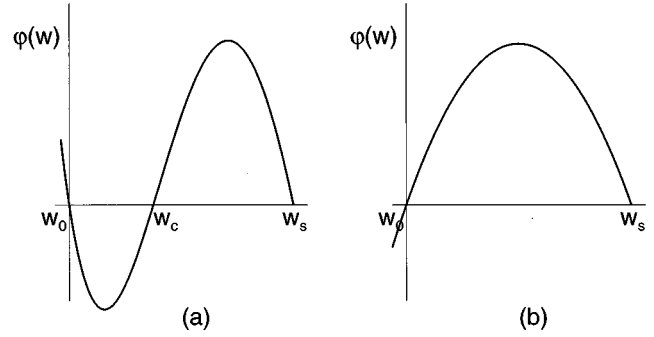

FIG. 4. The form of $\varphi(w)$ in Eq. (9) for two distinct regimes in the mean-field-like model. (a) The nucleation (metastable) regime; (b) the spinodal (unstable) regime.

We now need to choose an appropriate form for $\varphi(w)$. We assume at $t=0$ there is a nucleus of reconstructed facet around $y=0$ and as y goes to $\pm\infty$ the surface is uniform with $w=w_0$, the average terrace width. The main features of $\varphi(w)$ can be deduced using the reconstruction-driven faceting of Si(111) as an example. Figure 4 draws two postulated forms for $\varphi(w)$ in the nucleation and unstable regime, respectively. In the nucleation regime [Fig. 4(a)] the uniform surface is *metastable*. Thus we set $\varphi(w_0)=0$ and $\varphi'(w_0)<0$. (This ensures that w_0 is a stable fixed point.) However, when the facet width is larger than a certain critical width w_c, the effect of reconstruction will overcome the step repulsions and it will be energetically more favorable to increase the facet width. Thus $\varphi(w)$ becomes positive for $w>w_c$. As w further increases, the number of unreconstructed bunched steps around the facet becomes larger, slowing down the facet growth. Thus $\varphi(w)$ should decrease. For example, in Mullins's one-dimensional continuum model, the long time behavior of the facet width is $t^{1/2}$ and $t^{1/4}$ for the evaporation-condensation mechanism, and surface diffusion mechanism respectively, corresponding to w^{-1} and w^{-3} behavior for $\varphi(w)$ at large w. It was also observed for Si(111) that facet widths can saturate at certain values due to elastic effects.[16,17] This can be incorporated in our model by requiring that $\varphi(w)$ have another stable fixed point w_s at the appropriate distance. In the case considered by Mullins w_s is infinite. The discussion that follows does not depend on whether w_s is finite or not.

When we lower the quenching temperature, there is a crossover from metastable to unstable phase separation for Si(111).[16] Figure 4(b) draws the postulated form for $\varphi(w)$ for the *unstable* case. Here w_0 is still a fixed point but is unstable $[\varphi'(w_0)>0]$ and there is no intermediate fixed point w_c.

With this approximation for the ''driving force,'' and neglecting thermal noise, the problem of facet growth from a preexisting nucleus is reduced to the problem of solving the time evolution of Eq. (9) starting from some initial condition. The nonlinear term $\varphi(w)$ satisfies $\varphi(w_0)=\varphi(w_s)=0$. This problem has been thoroughly investigated by Aronson and Weinberger[38,39] as a model for population genetics. They have shown that the solution $w(y,t)$ of Eq. (9) will develop a stable profile that propagates with a well defined nonnegative steady-state velocity v_y for *any* continuous function
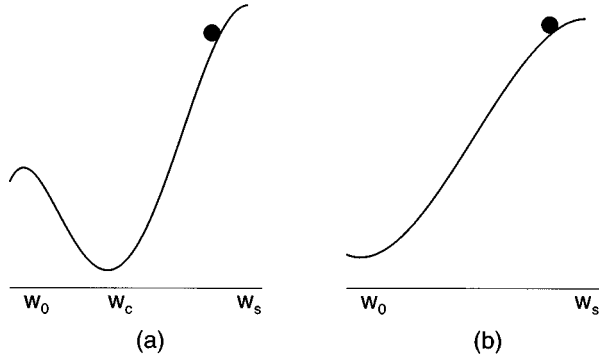
FIG. 5. The potential field for the particle whose trajectory represents a solution of the shape preserving equation. The fixed points now are shown as potential maximum and minimum. (a) and (b) correspond to the same regime as in Fig. 4.

$\varphi(w)$ defined on $[w_0,w_s]$ for which $\varphi(w_0)=\varphi(w_s)=0$, provided that the initial profile satisfies $w(y,0)\rightarrow w_0$ as $y\rightarrow\infty$ (i.e., far away from the nucleus the steps remain at their initial average positions), and that the nucleus is sufficiently localized. In other words, there exists one steady-state solution for the tip shape and velocity of the growing facet independent of most initial conditions of the nucleus.

To see this more clearly, let us consider shape preserving solutions of the form $w(y-ct)$, where c is a non-negative number that describes the propagation velocity of the profile in y direction. Then $w(\xi)=w(y-ct)$ satisfies

$$\gamma w'' + cw' + \varphi(w) = 0. \qquad (10)$$

We are only interested in $w(\xi)$ that satisfies $w(\xi)\neq w_0$ and $\lim_{\xi\rightarrow+\infty}w(\xi)=w_0$. To see that the steady state solution exists for a range of c's we follow the argument of Dee and Langer.[40] Equation (10) describes the trajectory of a particle of mass γ whose ''displacement'' w is a function of ''time'' ξ. The particle moves in a force field described by $-\varphi(w)$. Figure 5 illustrates this potential field for the two types of driving ''force'' $\varphi(w)$. Notice that a stable fixed point for Eq. (9) corresponds to a local potential maximum and an unstable fixed point corresponds to a local potential minimum. If c is positive, it serves as a damping coefficient and the damping force is proportional to the ''velocity'' $(\partial w/\partial\xi)$ of the particle. The relevant solution of our problem is a ''trajectory'' that starts from $w=w_s$ and ends at $w=w_0$. If c is very large, the particle is overdamped in the sense that starting from $w=w_s$ with an arbitrarily small velocity, the particle will either never reach $w=w_0$ [Fig. 5(a)] or approach $w=w_0$ monotonically [Fig. 5(b)]. On the other hand, if c is very small then the particle is underdamped and it will go past $w=w_0$ with a nonzero velocity. There exists a unique c^* such that the relevant trajectory is neither overdamped $(c>c^*)$, nor underdamped $(c<c^*)$. It can also be shown that c^* is the selected velocity if the system develops a stable profile starting from a localized initial nucleus.[38,39]

If $\varphi'(w_0)>0$, then the facet with average terrace width w_0 is *unstable*. For a variety of nonlinear functions $\varphi(w)$, the linear expansion around w_0 is enough to determine the velocity of the propagation of the profile along the y direction. This is a special case of the marginal stability mechanism of velocity selection.[40,41] In this case $v_y=c^*$ is simply $2(\gamma\varphi'(w_0))^{1/2}$. Stewart and Goldenfeld[42] have proposed a continuum model for the unstable regime. As an approximation, they also used this model to predict the traveling velocity of the facet in y direction. However, as pointed out by them and other authors, Si(111) quenched 3 °C below the transition temperature is not in an unstable regime. Rather phase separation proceeds through a nucleation and growth process. Therefore in the model we described above, we assumed terraces with $w=w_0$ are *metastable* and there is a threshold effect characterized by w_c.

In general the value of selected velocity v_y should depend on the behavior of $\varphi(w)$ through all w in the range of $[w_0,w_s]$. Here as an example of the relative effect of w_c and w_s, we use a simple form of φ that mimics the faceting problem, namely,

$$\varphi(w)=\begin{cases} 0, & w_0\leq w<w_c \text{ and } w>w_s \\ \varphi_0, & w_c\leq w\leq w_s. \end{cases} \qquad (11)$$

The important parameters are the critical width w_c for the formation of the reconstruction, and φ_0, which mimics the effect of the reconstruction on the motion of the step in x direction. This of course is an unrealistic form for $\varphi(w)$ but still qualitatively representative. It can be shown by solving Eq. (10) explicitly that the steady-state velocity v_y that is selected dynamically satisfies the following equation:

$$v_y^2 = \frac{\gamma\varphi_0}{w_c-w_0}\{1-\exp[-v_y^2(w_s-w_0)/\gamma\varphi_0]\}. \qquad (12)$$

For $w_s/w_c\gg 1$, $v_y\approx[\gamma\varphi_0/(w_c-w_0)]^{1/2}$. Here we have a relation between the growth rate of the facet in the two directions. The result that the facet propagates with a constant velocity in the y direction is rather insensitive to the choice of $\varphi(w)$. In order for the facet to grow in area, the positive part of $\varphi(w)$ should be large enough so that

$$\int_{w_0}^{w_s} dw \; \varphi(w)>0. \qquad (13)$$

Although this mean-field model is too simple to predict the evolution of the nucleation quantitatively, it does reproduce some of the essential features of the TSK model. Equation (12) also qualitatively predicts correctly the trends when changing the parameters involved.

IV. NUMERICAL CALCULATION AND COMPARISON WITH EXPERIMENT

We now return to a study of the general coupled step equations derived in Sec. II. Phaneuf *et al.*[16] have studied the reconstruction-induced phase separation of vicinal Si(111) using low-energy electron microscopy. They found that below some transition temperature, large (7×7) facets form and in between these facets are unreconstructed step bunches. Depending upon how far the temperature was quenched below the transition temperature, the evolution toward the final state was quite different. For example, for the surface with 4° miscut (with average terrace width $w_0=49$ Å) quenched 3 °C below the transition temperature, the facet formation occurs by the nucleation and growth of

isolated linear (7×7) reconstructed (111) facets. For quenches to lower temperatures, many facets appeared simultaneously. This change of kinetics has been associated with a change from nucleation and growth to spinodal decomposition.[32] Recent scanning tunneling microscope (STM) work using dc current heating reproduces most of these results.[19]

The thermodynamics of vicinal Si(111) surfaces has been discussed at length in Refs. 11 and 12. The variation with temperature in the difference of surface free energy density for the two phases $\Delta f^0 = f_u^0 - f_r^0$ can be determined from the phase diagram of the faceting. Using the tie-bar construction in Fig. 2 we have $s_b = (\Delta f^0/2g_u h^3)^{1/3}$, where s_b is the final step density of the unreconstructed step bunch. Using $g_u = 15$ meV/Å^2,[11,12] we estimate $\Delta f^0 \approx 0.02$ meV/Å^2 at 3 °C below the transition temperature for surfaces with 4° miscut. The difference in step creation energy $\Delta\beta = \beta_r - \beta_u$ cannot be determined exactly from the phase diagram and we use the estimate $\Delta\beta = 2$ meV/Å.[32] The critical width w_c corresponds to the intersection of the two free energy curves and is given by $\Delta\beta/\Delta f^0$. Using these values w_c is estimated around 100 Å, which is consistent with the STM study by Hibino, Homma, and Ogino.[19] Henceforth we use $w_c = 2w_0 = 98$ Å.

The kinetic coefficients can be obtained from the measurements of thermal fluctuations of the steps. For surfaces with very small miscut angle, we can ignore the repulsive interaction terms in the step edge chemical potential. Assuming the attachment/detachment mechanism and the equilibrium chemical potential value on terraces, the equation of motion of the step is simply

$$\frac{\partial x(y)}{\partial t} = 2\alpha\Omega^2\widetilde{\beta}\frac{\partial^2 x}{\partial y^2} = \frac{\Gamma\widetilde{\beta}}{k_B T}\frac{\partial^2 x}{\partial y^2}. \tag{14}$$

The last equation on the right is the deterministic part of the Langevin equation analyzed by Bartelt et al.[37] This allows us to identify $2k_B T\alpha\Omega^2$ with Γ, the mobility of the step wandering. Experiments at 900 °C show that $\Gamma = 5\times10^7$ Å^3 s^{-1} and $\widetilde{\beta} = 30$ meV/Å.[37] Note that in the analysis of the thermal fluctuations, the step is also coarse grained along the y direction, so there is no inherent microscopic length scale in these parameters.

To simulate the experiment discussed earlier, we manually create a nucleus of a wide reconstructed terrace (facet) in a system of 40 steps with average terrace width $w_0 = 49$ Å, and then calculate the deterministic time evolution of the facet by numerically integrating Eq. (7) or (8). The nucleus has a width larger than the critical width w_c and several steps near the nucleus are moved away from their uniform position to prevent overhangs. Far away from the nucleus, the steps are uniform. If the initial nucleus is big enough, the facet will continue to grow in size. In both the conserved and nonconserved cases we found a constant growth rate in y direction and a decreasing growth rate in x direction after a short transient. Figure 6 is a snapshot of the evolution of the surface profile using the locally conserved mechanism [Eq. (7)]. In this case, the growth rate in the y direction, v_y, is 830 Å/s, remarkably close to the experimental value 1000±200Å/s.[16] The good agreement is somewhat fortuitous, since the result is rather sensitive to several parameters
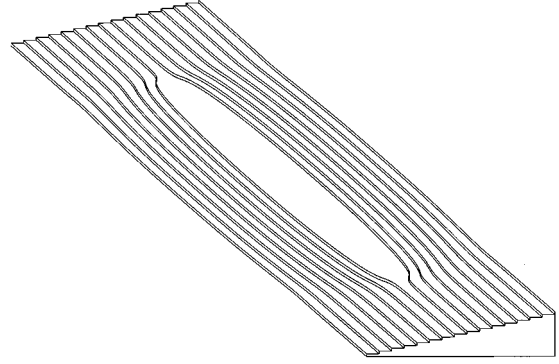

FIG. 6. A snapshot of a system of 40 steps after about 4 s starting from a small nucleus using the local conservation mechanism. Some of the parameters used are $g = 15$ meV/Å^2, $\Delta f^0 = 0.020$ meV/Å^2, $\Gamma = 5\times10^7$ Å^3/s, $w_0 = 49$ Å, and $w_c = 98$ Å.

that are not known accurately, especially the critical width w_c (or equivalently $\Delta\beta$). For example, for w_c equal to $1.7w_0$ and to $2.3w_0$, the corresponding v_y is 2400 Å/s and 350 Å/s, respectively. However, the nonlocally conserved mechanism with Eq. (8), assuming $w_c = 100$ Å, gives $v_y = 2.0\times10^4$ Å/s, about 20 times larger than experiment.

Although it is difficult to estimate the uncertainty of v_y without a more detailed knowledge of w_c, these results suggest that the mechanism with local conservation is probably a more realistic scenario for Si(111) at this temperature. Recent experiments on the relaxation of one-dimensional Si(111) step bunches are also consistent with the locally conserved mechanism.[24]

However, as remarked earlier, the local conservation condition is more questionable in a two-dimensional system if we also consider diffusion of adatoms on terraces along the step edge direction. Let d_y be the typical distance an adatom diffuses on the terrace along the y direction before it attaches to the steps. The variation in the y direction of the atom chemical potential on terraces with wavelengths much smaller than d_y will be smoothed out by diffusion before it has any effect on step motion. When d_y is much larger than the largest relevant length scales, for example, the distance between different facets or the size of the facet, the nonlocally conserved mechanism will be more realistic. In the limit that d_y is small compared to the length scale on which the steps have features we are interested in, the diffusion problem is essentially one dimensional and the locally conserved mechanism is more realistic, provided there is no direct adatom hopping between different terraces. If we denote D_s as the adatom diffusion rate on the terrace and c_{eq} as the equilibrium adatom concentration, then d_y is of the order of $(D_s c_{eq}\Omega^2 w_0/\Gamma)^{1/2}$, assuming isotropic diffusion. This yields an estimate for d_y of 500 Å using[43] $D_s c_{eq} = 1.2\times10^9$s^{-1}. This length is much smaller than the lateral size of the facets and is comparable to the size of the tip. Thus it clearly rules out the nonlocally conserved mechanism for facet widening. This can be viewed as an independent argument for choosing the locally conserved mechanism aside from the fact that the v_y it gives is much closer to the experimental value. A quantitative description of the crossover regime near the tip where

d_y has an intermediate value necessarily involves two-dimensional diffusion of adatoms and is beyond the scope of this paper.

V. CONCLUSION

In this paper we have proposed two self-consistent numerical models for the motion of steps on a vicinal surface under a reconstructive phase transition. We found a steady facet front propagation in the direction parallel to the step edges as has been observed experimentally. The underlying mechanism for the velocity selection is believed to be the balance of the stabilizing effect of the line tension and the driving force arising from phase separation due to the surface reconstruction. Using thermodynamic parameters obtained mostly from equilibrium fluctuation measurements and the Si(111) reconstruction phase diagram, we obtain a satisfactory agreement of the model with experimental data using the mechanism requiring local conservation of adatoms on each terrace. More accurate experimental measurements of the relevant parameters will allow a more detailed understanding of the microscopic mechanisms.

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