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The equilibration of terrace width distributions on stepped surfaces

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Many recent attempts to understand step structure have been based on the assumption of thermal equilibrium. In order to aid such analyses, we present calculations of the order of magnitudes of equilibration times for step structure. In particular, we discuss the equilibration of the distribution of terrace widths when step motion occurs through the exchange of atoms with a reservoir of adatoms on the terraces. By solving the appropriate continuum Langevin equation we give simple expressions for the time dependence of the terrace width distribution in terms of attachment/detachment rates at the step edge. We show that equilibration times should scale as the fourth power of the equilibrium width of the distribution (which can usually be expected to be proportional to the average terrace width). We verify this prediction for a discrete model of step dynamics with a Monte Carlo simulation. When equilibration occurs only through diffusion along the step edge, the equilibration times are much longer: they scale as the eighth power of the equilibrium width.

1. Introduction

Since the structure of steps on surfaces influences many surface processes, it is important to understand the microscopic mechanisms responsible for step configurations. Recently there have been a few attempts to interpret step structure in terms of *equilibrium* statistical mechanical models [1–4]. One of the most difficult aspects of this type of interpretation is the question of whether, or at what temperature, thermal equilibrium has been achieved.

Single-crystal surfaces, in their processing, almost certainly pass through stages which take their step structure out of equilibrium. We have in mind, in particular, the intensely studied surfaces of Si which are often cleaned by heating to temperatures where considerable sublimation, and thus step motion, occurs. The kinetics of step motion can create step configurations which are very far from equilibrium [5] – in principle even changing the average height of steps [6]. Whether surface diffusion at any particular temperature is large enough to bring such non-equilibrium configurations into equilibrium is a very difficult issue on which to make general pronouncements. For example, even the diffusion of single atoms on terraces is not generally well characterized. Evaluating equilibration is a particularly severe problem in interpreting measurements in which one cannot monitor the temperature evolution, such as room-temperature STM [1,2,7].

To address this problem, we consider several simple models of the time dependence of one particular feature of stepped surfaces: the distribution of terrace widths. Since equilibrium terrace width distributions are strongly influenced by the interactions between steps [8,9], their measurement has proven to be a useful tool in checking theories of step–step interactions [1,3,4,7]. Terrace width distributions have also been used as a tool for characterizing surfaces grown by molecular beam epitaxy [10]. There are, naturally, many ways in which terrace width distributions can be out of equilibrium. Rather than try to anticipate all the various ways, here we consider the simple possibility of initially straight and equidistant steps, and inquire about the times required for the thermally induced meandering of the steps to equilibrate the terrace width distribu-

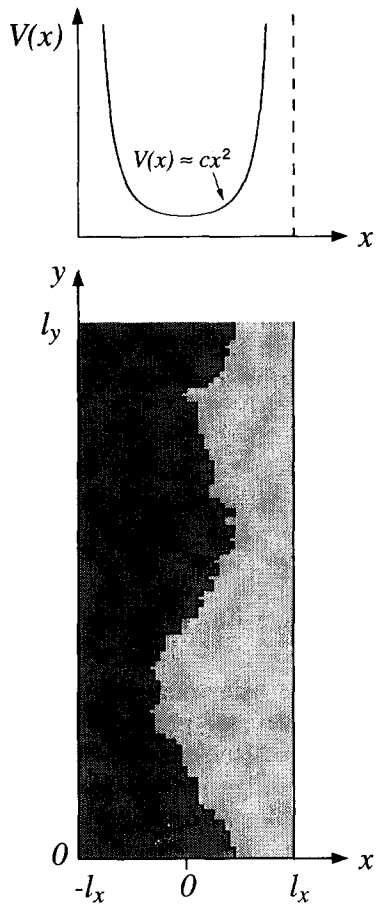

Fig. 1. The coordinate system and step geometry used in this paper. In section 2 we consider a step confined by a quadratic potential $V(x)$; in section 3 we also consider a step constrained between two parallel walls (the Gruber–Mullins model).

tions. This scenario is not as academic as it might appear: sublimation or growth effects can create terrace width distributions narrower than equilibrium [6]. Extensions to other situations are not difficult.

Equilibrium terrace width distributions are determined by a balance between the entropy gained by step wandering and the (energetic) repulsions between neighboring steps. Constraining a step to a narrow region (see fig. 1) costs entropy. To estimate the magnitude of this loss – the motivation for subsequent broadening to the equilibrium width – we recall the arguments of Fisher and Fisher [11] for the case in which a step is freely wandering between two adjacent steps, with only the constraint that steps cannot cross. In this picture, each step–step collision decreases the number of the configurations available per step by a factor of two: thus each step–step collision costs entropy on the order of $k_B \ln 2$. The number of collisions can be estimated from the fact that a step will wander on the order of a terrace width l in a distance $y \approx a_{\parallel} l^2/b^2$, where b^2 is the mean square size of each kink, and $a_{\parallel}$ is the distance between possible kink sites. Thus the free energy increase per lattice constant along the step is approximately $k_B T b^2 (\ln 2)/a_{\parallel} l^2$. (More rigorous calculations are readily available which substantiate this estimate [11].) Taking the relatively large value of $b = 1.4 a_{\perp}$ (as observed experimentally for single-layer height steps on vicinal Si(100) [2]), would imply a free energy increase of only approximately $k_B T/100$ per step-edge site for restricting the terraces to have widths within 10 lattice constants of each other (the width observed for Si(100) misoriented by 1° towards the [110] direction). Whether such a small free energy decrease is sufficient motivation for the wandering of a step to equilibrate in a reasonable length of time is a serious question, especially considering the large amount of mass transport required for step movement. It is the question which is addressed in this paper.

The form of the terrace width distributions depends on the magnitude of the energetic interactions between steps. As in previous work on equilibrium distributions [8], we will model the constraining influence of these interactions with a quadratic potential. For interactions which fall off like the inverse square of the separation between steps (as one usually expects [12]), the width of the distributions is proportional to the average terrace width, as it is for the case when there are no energetic interactions. As we will discuss, the equilibration times increase markedly with increasing average terrace width.

To model the kinetics of the step wandering, we initially follow the spirit of the classic Burton–Cabrera–Frank model [13] of step motion in crystal growth. We suppose that on the terraces separating the steps there is a supply of

adatoms which are in equilibrium with the step (kink) sites. We use two calculational approaches on this model. In the first, we solve the appropriate continuum Langevin equation governing equilibration, which allows us to write down analytic equations for the time dependence of the step structure. In the second, we perform a simple Monte Carlo calculation on a discrete lattice to determine the regime of validity of the continuum approach and to show explicitly how the parameters of the continuum approach are related to atomic motion.

An obvious alternative model, considered briefly at the end of this paper, is that steps wander only by exchanging atoms along their length: this, as we discuss, naturally leads to a much slower asymptotic equilibration.

2. Langevin dynamics

In the Langevin formalism, each degree of freedom of the step is assumed to diffuse towards lower energy with a speed proportional to the gradient in the energy, subject to thermal fluctuations. We assume that x can be described as a continuous function of y and try to describe positions of the step edge separated by more than a few lattice constants. The step dynamics are then governed by

$$\frac{\partial x}{\partial t} = -\frac{\Gamma_a}{k_B T}\frac{\delta H}{\delta x} + \eta(y, t). \tag{1}$$

The noise term η allows for thermal fluctuations. As we discuss shortly, the "friction" coefficient Γ_a depends on the size and nature of η. The appropriateness of this equation relies on the assumption that at least small segments of the step edge are in equilibrium – e.g., the kink density is close to the equilibrium value. This assumption is a reasonable one to make if we are interested in the evolution of the terrace width distribution – it is likely that quantities such as the kink density would equilibrate much sooner than the terrace width distribution, for example. We suppose that the noise is uncorrelated and characterize its strength by a time τ_a:

$$\langle \eta(y, t)\eta(y', t')\rangle = 2\frac{a_\perp^2 a_\parallel}{\tau_a}\delta(t - t')\delta(y - y'), \tag{2}$$

where $a_\perp$ and $a_\parallel$ are lattice constants perpendicular and parallel to the step edge. We expect that τ_a will be, at least roughly, the time between adatom attachments/detachments at the step edge (an expectation verified in the following section). One can show [14,15] that for eqs. (1) and (2) to describe an approach to equilibrium, we must have

$$\Gamma_a = a_\perp^2 a_\parallel/\tau_a. \tag{3}$$

In the coarse-grained picture of eq. (1), the effective Hamiltonian can be approximated by

$$H = \int \left[\tfrac{1}{2}\tilde{\gamma}\left(\frac{\partial x}{\partial y}\right)^2 + V(x)\right] \mathrm{d}y, \tag{4}$$

where $\tilde{\gamma}$ is the "step-edge stiffness" [16], and $V(x)$ is the (average) potential field (per unit length) which the step experiences due to other steps. The step-edge stiffness is related to the mean square kink size b^2 described in the introduction through [8,17]

$$\tilde{\gamma} = \frac{k_B T a_\parallel}{b^2(T)}. \tag{5}$$

Thus, in high-symmetry directions $\tilde{\gamma}$ usually diverges as T approaches zero. For concreteness in what follows, we will assume that the step is confined close to $x = 0$ by a potential of the form $V(x) = cx^2$ (see fig. 1). This model can very accurately describe terrace width distributions for many interacting steps [8,9]. With eq. (4) and this choice of potential, eq. (1) can be written as [18,19]

$$\frac{\partial x}{\partial t} = \frac{\Gamma_a \tilde{\gamma}}{k_B T}\left(\frac{\partial^2 x}{\partial y^2}\right) - \frac{2c\Gamma_a x}{k_B T} + \eta(y, t). \tag{6}$$

This type of equation [2] has been the subject of much investigation: because it is linear in x, expectation values can be easily found by Fourier transformation [21,23]. In thermal equilibrium (at large times), it can be easily shown [8] that the

probability of a step to be at position x is just

$$P(x) = \frac{1}{w_\infty \sqrt{2\pi}} \exp(-x^2/2w_\infty^2), \tag{7}$$

where the equilibrium width w_∞ is

$$w_\infty^2 = \frac{k_B T}{\sqrt{8c\tilde{\gamma}}}. \tag{8}$$

We are interested in the time dependence of the root-mean-square width of the terrace width distribution, $w(t)$. In order to estimate the equilibration times, we suppose the step is initially straight, and compute the time evolution of the width w of the terrace width distribution. From eq. (6), we find

$$w^2(t) = \langle x^2(t) \rangle = w_\infty^2 \operatorname{erf}\left(\sqrt{\frac{2t}{\tau_{eq}}} \right), \tag{9}$$

where the time τ_{eq},

$$\tau_{eq} = \frac{k_B T}{2c\Gamma_a} = \frac{4w_\infty^4 \tilde{\gamma}}{k_B T \Gamma_a}, \tag{10}$$

is a measure of the equilibration time: when $t = \tau_{eq}$, w has reached 98% of its final value. Expansion of the error function at small t, where the constraining potential is not yet felt, gives

$$w(t) = \left(\frac{2k_B T \Gamma_a t}{\pi \tilde{\gamma}} \right)^{1/4}. \tag{11}$$

Eqs. (9) and (10) show that the time dependence of the terrace width distribution scales as the fourth power of w_∞ (which is usually proportional to the average distance between steps [8]). As an example of the quantitative use of these equations, we consider the case of Si(111): Alfonso et al. [4] have measured terrace width distributions at 900°C using reflection electron microscopy. From measurement of the mean square meanderings of isolated step edges, they determined $\tilde{\gamma}$ to be approximately 1.1×10^{-5} erg cm^{-1}. For the observed value of $w(t)$ of 200 Å (when the average terrace width is 600 Å) to represent 90% of the equilibrium value after, say, an hour of equilibration, eq. (9) would require that τ_a should be on the order of 10^{-3} s (assuming single-atom step attachment–detachment). If such rapid attachment was actually occurring, then small-scale temporal fluctuations in step edge position should be readily observable (for an example, see ref. [24]). An estimate of these fluctuations can be found by noting that the *equilibrium* fluctuations of eq. (6) are governed by an expression similar to eq. (9):

$$\langle x^2(t) \rangle - \langle x(t)x(t') \rangle = w_\infty^2 \operatorname{erf}\left(\sqrt{\frac{2|t-t'|}{\tau_{eq}}} \right). \tag{12}$$

Using the parameters obtained for Si(111) by Alfonso et al. in this equation, one finds that equilibration times of one hour are associated with equilibrium fluctuations of the order of 20 Å every second in the position of the step edge at any particular y. These fluctuations, should, in principle, be observable.

Next, we discuss the relationship between the rate of change of the amount of step meandering contained in eq. (9), and changes in the average position of the step. It is easy to show from eq. (6), that if a step initially has a mean position x_0 away from the equilibrium position at $x = 0$, then the mean position will approach equilibrium as

$$\langle x \rangle = x_0 \exp(-t/\tau_{eq}), \tag{13}$$

with τ_{eq} given by eq. (10). Relaxations to equilibrium of the form of eq. (13) have been observed experimentally on vicinal Si(001) surfaces after the removal of an externally applied strain [7,25]. (We mention in passing that eq. (13) has also been derived in ref. [7] with, however, a different expression for τ_{eq} – in our model τ_{eq} does not depend explicitly upon $\tilde{\gamma}$ – i.e., kink energies [26].) Significantly, τ_{eq} governs *both* the equilibration of the average step edge position and the terrace width distribution. Thus, given the experimental observations of Webb [7] of the equilibration of the average step position on Si(001), one can be very optimistic that the reported terrace width distributions are also in equilibrium (despite the small driving forces discussed in section 1!). The value of 40 s for τ_{eq} reported for terraces on Si(001) separated by 260 Å at 550°C, corresponds to a value of τ_a of 3×10^{-4} s, taking $a_\perp$

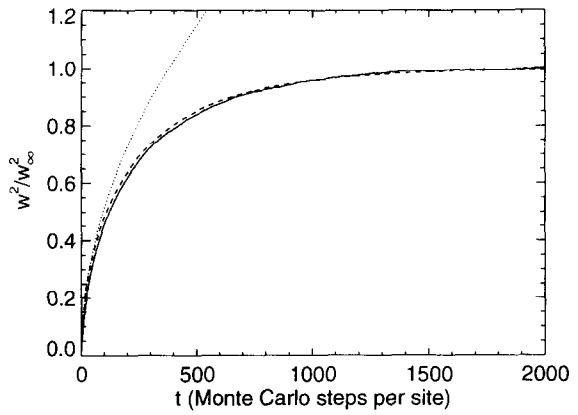

Fig. 2. The time dependence of w, the root-mean-square width of the terrace width distribution, from a Monte Carlo simulation of an *isolated* step which is initially straight. At long times, w approaches the equilibrium value w_∞ determined by the strength of the constraining potential. The dashed line shows the prediction of eq. (9): the dotted line shows the early time behavior of eq. (11). The temperature is equal to the kink energy ϵk_B.

and $a_\parallel$ to be the observed kink dimensions of 7.7 Å.

3. Monte Carlo dynamics

The Langevin approach of the preceding section is phenomenological. Although very plausible, there is generally no way of deriving eq. (1) directly from a microscopic model of the kinetics. To check how the features of the Langevin prediction of eq. (9) are realized in an atomic model of step motion, we have have used standard Monte Carlo techniques [27] to study the equilibration kinetics of a step composed of kinks of length $na_\perp$ costing energy $n\epsilon$. Fig. 2 shows the time dependence of the width w of the terrace width distribution for $k_BT = \epsilon$ and weakly interacting steps with $c = 0.002k_BT/a_\perp^2 a_\parallel$. In the simulation, periodic boundary conditions were used in the y direction: l_y was taken to be $200a_\parallel$. Points along the step were randomly chosen: the Monte Carlo unit of time is defined as l_y such trials. For each selected step site, we tried to add or subtract an atom according to the standard Metropolis Monte Carlo algorithm. In calculating fig. 2, 1000 runs were averaged. To check if the behavior of fig. 2 is consistent with eq. (9) we need to know Γ_a: we thus kept track of the frequency of changes in the kink structure. At this temperature, the probability that any particular site is changed during a single Monte Carlo step was 0.267 [28]: we thus make the identification $\tau_a = 1/0.267 \approx 3.7$, where time is measured in units of Monte Carlo steps per site. For the simulated model, $b^2(T) = a_\perp^2/(2\sinh^2(\epsilon/2k_BT))$, so that $b^2(T=\epsilon) \approx 1.84a_\perp^2$. Using eq. (8), this gives $w_\infty = 3.27a_\perp$, which compared well with the observed value of $w_\infty = 3.20a_\perp$. The dashed line in fig. 2 shows the prediction of eq. (9): the agreement is good: thus the continuum approach of the preceding section provides a useful description of the kinetics of our (atomic scale) simulation!

The dotted line in fig. 2 compared the short-time behavior predicted by eq. (11) with the simulation results. Deviations from eq. (11) quickly occur because of the comparatively small value of w_∞. To study the short-time regime more thoroughly, we also simulated the case of non-interacting steps, i.e., $c = 0$: the results are shown in

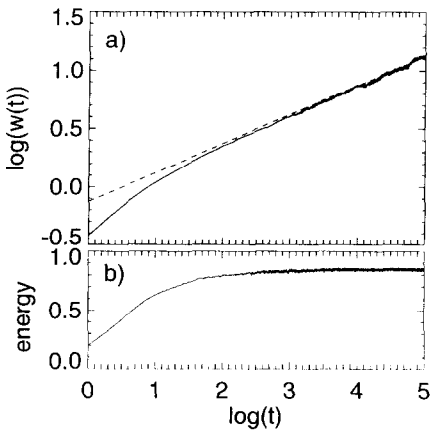

Fig. 3. (a) A log–log plot of the time dependence of w for the case of no constraining potential. The dashed line is the curve $w = 0.75a_\perp t^{1/4}$, the form expected from eq. (11). (b) The time dependence of the energy (per kink site) of the step showing that the very short time transient of (a) is associated with the equilibration of the local kink structure. Energy is in units of the kink energy ϵ, and time is in unit of Monte Carlo steps per site.

fig. 3a. Substituting eq. (5) into eq. (11), we expect

$$w(t) \approx 0.75 a_\perp t^{1/4}, \tag{14}$$

with time again measured in units of Monte Carlo steps per site. This prediction is compared with our simulation in fig. 3a: after a short time transient, the $t^{1/4}$ prediction of eq. (14) described the data well: even the amplitude of the power law is in reasonable accord with the Monte Carlo calculation. As shown by fig. 3b, the short time transient is a measure of the equilibration of the local kink structure: deviations from the $t^{1/4}$ behavior only occur when the energy of the step is substantially different from its equilibrium value [29]. (That the energy equilibrates so rapidly suggests that for analyses of STM data for kink energies [2,30], equilibration should be of much less concern compared to terrace width distributions.)

To show that the general features of eq. (9) are independent of the particular model of the preceding section (in particular the choice of a quadratic potential), we have also studied with Monte Carlo simulations the model introduced by Gruber and Mullins [31]. A single step is confined between two straight walls separated by twice the average step spacing $2l_x$ (see fig. 1). This model again neglects the possible complexity of step collisions, but still accurately described

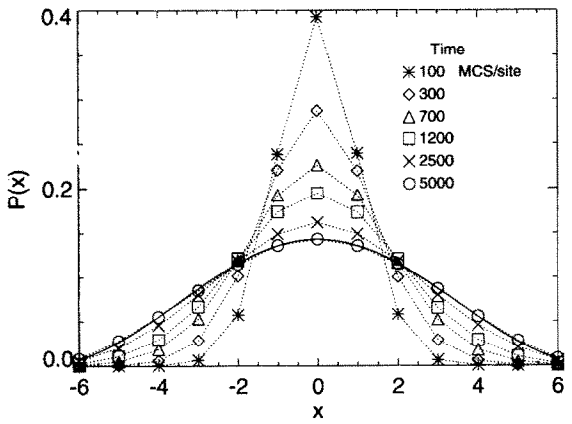

Fig. 4. Monte Carlo results (points connected by dashed lines) for the time evolution terrace width distribution $P(x)$ for the Gruber–Mullins model with l_x equal to 13 lattice constants. The solid line shows the equilibrium distribution of eq. (15).

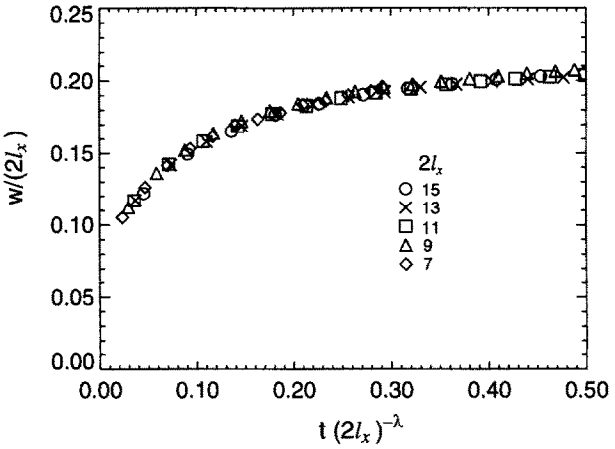

Fig. 5. Plot of the time dependence of the width of terrace width distributions for various L, scaled according to eq. (16), with $\lambda = 3.6$.

the terrace width distributions for non-interacting steps. Compared with the quadratic constraining potential, this model is more appropriate for steps without energetic interactions (it differs from the $c = 0$ case of the preceding paragraph because of the possibility of collisions of the steps with the walls). When l_x is large compared to b, the probability that the step is found a distance x from the midpoint between the walls is just

$$P(x) = \frac{1}{l_x}\cos^2\left(\frac{\pi x}{2l_x}\right). \tag{15}$$

From eq. (9) we expect the width of the terrace width distribution to have the scaling form (using the fact that $w_\infty \propto l_x$ for the Gruber–Mullins model):

$$w(t) = l_x G\left(t/l_x^\lambda\right). \tag{16}$$

where the scaling function $G(u)$ will be different from that given in eq. (9), because of the differences of eq. (15) from eq. (7). To check the validity of this equation, we examined the time dependence of w for $2l_x = 7$, 9, 11, 13 and $15a_\perp$. Fig. 4 shows the evolution of the terrace width distribution for $2l_x = 13$. Fig. 5 shows the plot scaled according to eq. (16): the best fit λ is ~ 3.6, close to the value of 4 anticipated from eqs. (9) and (10). Given the relatively small l_x values considered, 10% deviation seems a reasonable agreement.

4. The case when diffusion is restricted to the step edge

If the temperature is low, one might expect the density of diffusing adatoms on terraces to be extremely low, so that step motion can occur most easily through atoms diffusing along the step edge. (Rapid diffusion along step edges has been observed to occur even at room temperature on stepped Ag(111) [3,24].) In this situation, one can expect a much slower approach to equilibrium. When mass transport occurs only along the step edge, there is a constraint that the integral over x is fixed. The analog of eq. (6) can then be shown to be ("Model B" of ref. [14]):

$$\frac{\partial x}{\partial t} = \frac{\Gamma_h \tilde{\gamma}}{k_B T}\frac{\partial^4 x}{\partial y^4} - \frac{2c\Gamma_h}{k_B T}\frac{\partial^2 x}{\partial y^2} + \eta(y, t), \qquad (17)$$

where now the noise term must be correlated because atoms are hopping from one site to another:

$$\langle \eta(y, t)\eta(y', t')\rangle = 2\Gamma_h \delta(t - t')\delta''(y - y'). \qquad (18)$$

If the step diffuses by atoms hopping one lattice constant per time τ_h, then we identify

$$\Gamma_h = \frac{a_\parallel^3 a_\perp^2}{\tau_h}. \qquad (19)$$

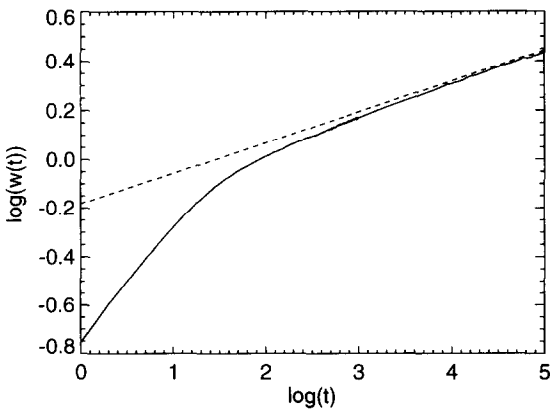

Fig. 6. A log–log plot of the time dependence of the root-mean-square width of the terrace width distribution from a Monte Carlo simulation of an *isolated* step evolving through step-edge diffusion. The dashed line shows the theory of eq. (22), i.e., $w \propto t^{1/8}$.

Eq. (17) is again linear in x and thus the expectation values can be found by Fourier transformation. The result is

$$w^2(t) = w_\infty^2 F\left(\frac{(k_B T)^3 \Gamma_h t}{64\tilde{\gamma}^3 w_\infty^8}\right). \qquad (20)$$

with the scaling function $F(v)$ given by

$$F(v) = \frac{\sqrt{8}}{\pi} v^{1/4} \int_0^\infty du \frac{1 - \exp(-2u^4)}{u^2 + 2\sqrt{v}}. \qquad (21)$$

Notice that now τ_{eq} of eq. (10) does not determine the equilibration time. At short times (before the effect of the constraining potential is felt) eq. (20) becomes

$$w^2 = \left(\frac{(k_B T)^3 \Gamma_h t}{\tilde{\gamma}^3}\right)^{1/4} \frac{1}{\pi}\int_0^\infty du \frac{1 - \exp(-2u^4)}{u^2}$$

$$\approx (0.46385\ldots)\left(\frac{(k_B T)^3 \Gamma_h t}{\tilde{\gamma}^3}\right)^{1/4}. \qquad (22)$$

Compared to eqs. (9) and (11), the equilibration of eqs. (20) and (22) is very much slower: in particular the equilibration times scale as the *eighth* (!) power of the terrace width distribution. In terms of the vicinal Si(111) example of section 2, eq. (20) [32] implies that equilibration to 90% of the terrace width distribution for $w_\infty = 200$ Å in one hour would require a value of τ_h in eq. (19) of around 10^{-13} s, which seems unphysically small.

Fig. 6 shows the results of a Monte Carlo simulation of an initially straight step evolving through step-edge diffusion at $k_B T = \epsilon$. The dashed line shows the $t^{1/8}$ behavior predicted from eq. (22), using the hop rate from the simulation ($\tau_h = 0.135$ Monte Carlo steps) to determine Γ_h. Again, aside from short transients (in which the local kink structure is equilibrating). Eq. (22) provides a good description of the observed behavior.

5. Conclusion

The principal result of this paper is the observation that equilibration times for terrace width distributions grow as fairly large powers of the

equilibrium width of the distribution: 4 for adatom attachment and 8 for step-edge diffusion. Thus, confirming the suspicion raised in the introduction, the entropy of step wandering can indeed be a small driving force for the diffusion towards equilibrium of widely spaced steps. For steps on the order of a few hundred ångströms apart to be in equilibrium at typical experimental temperatures requires on the order of 1000 adatom attachments/detachments at the step edge every second.

Another point we stress is that the large fluctuations needed to equilibrate widely separated steps are naturally associated with large *equilibrium* fluctuations (as, for example, comparison of eq. (9) with eq. (12) shows). If one is to hypothesize that steps are in equilibrium, it is important to check that the existence of these fluctuations is consistent with experimental observations.

We should point out that the above models have left out some physics which could in principle be important. The foremost among these deficiencies is that we have not considered the equilibration of the average position of *groups* of steps – a problem important in such problems as faceting and step height doubling transitions. We have neglected gradients in the adatom diffusion field near step edges. We have also implicitly assumed that the net number of atoms which are leaving the step edge is the same as those that attach (a consequence of the assumption of local equilibrium leading to eq. (3)). Finally, these equilibration times will probably drastically underestimate the equilibration of the logarithmetic divergence of the height–height correlation function. Despite these limitations, eqs. (9) and (20) at least provide a guideline for estimating orders of magnitude of important components to equilibration times in terms of attachment and hop rates at the step edge. (The problem of relating these rates to surface diffusion constants is discussed, for example, in ref. [7].)

Acknowledgements

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