Terrace-Width Distributions on Vicinal Surfaces: The Basics

T. L. Einstein
University of Maryland

In this nugget we present basic ideas about the terrace-width distribution (TWD) of a vicinal surfaces and the physics it reveals. This exposition is preparatory to subsequent nuggets with more advanced and recent findings.

The miscut angle ϕ of a vicinal surface fully determines the average spacing $\langle\lambda\rangle$ between steps: $\langle\lambda\rangle \propto 1/\tan(\phi)$. For a "perfect staircase", as illustrated in Fig. 1, each step-step spacing λ is $\langle\lambda\rangle$; in other words, the TWD is a delta function. Since $\langle\lambda\rangle$ is the only characteristic length in the "downstairs" direction (called x in "Maryland notation"), it is convenient to adopt a dimensionless length s, where $s \equiv \lambda/\langle\lambda\rangle$. Then $P(s) = \delta(s - 1)$. Such a configuration, which corresponds to the limit of infinite step stiffness and infinite step-step repulsion, is unlikely to occur in nature.

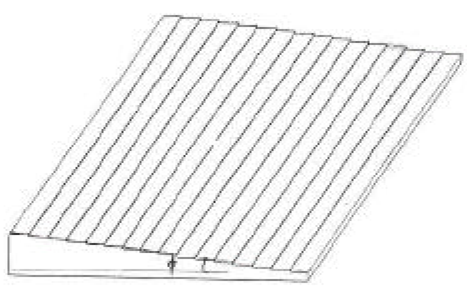

FIG. 1. Illustration of a "perfect staircase", for which $\lambda = \langle\lambda\rangle$ and $P(s) = \delta(s - 1)$.

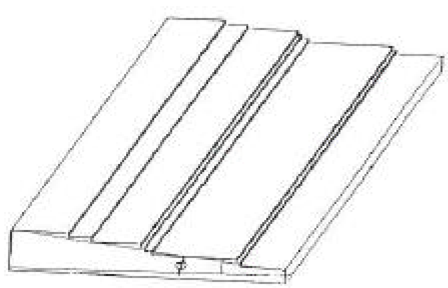

FIG. 2. Illustration of a stepped surface formed by straight steps dropped randomly, yielding $P(s) = \exp(-s)$.

A second simple possibility, illustrated in Fig. 2, is that the steps remain perfectly straight (like uncooked spaghetti, i.e. again the limit of infinite stiffness) but are placed randomly: If we take the unit spacing in the x direction to be a, then the probability of finding a step at any position is $a/\langle\lambda\rangle$, so that the probability of the step nearest a given step being n spacings away is $(1-a/\langle\lambda\rangle)^{n-1}(a/\langle\lambda\rangle)$. In the continuum limit, this distribution takes the exponential form $P(s) = \exp(-s)$. There are several steps that are close together along with many that are separated by much more than $\langle\lambda\rangle$.

On most vicinal surfaces one finds the sorts of configurations depicted in Fig. 3, with substantial meandering of the steps. That simulation was carried out for a terrace-step-kink model, in which the only thermal excitations are kinks on the step edges. (This is an excellent approximation at relatively low temperatures, since the excitation energy of a terrace "defect" atom or vacancy is several times that of a kink.)

FIG. 3. Illustration of a stepped surface with meandering steps, specifically a Monte Carlo simulation of the terrace-step-kink model.

The resulting form of $P(s)$ is depicted in Fig. 4, along with the TWD's for the two preceding cases. The most striking difference, seen also in the configuration shown in Fig. 3, is the dramatic decrease in the probability of finding terraces with widths much smaller than $\langle\lambda\rangle$. This decrease is attributed to an entropic or steric repulsion: Since steps cannot cross, a step that is near another step has fewer possibilities for meandering, and so contributes less to the free energy [1]. The resulting effective repulsion varies like λ^{-2}, just like the typical $A\lambda^{-2}$ elastic repulsion between steps [2]. (For the special case $A = 0$, depicted in Fig. 3, $P(s)$ can be very well described by a sequence of analytic approximants [2].)

In order that the mean of the TWD be preserved, the number of very broad terraces, with λ at least a few times $\langle\lambda\rangle$, is also suppressed.

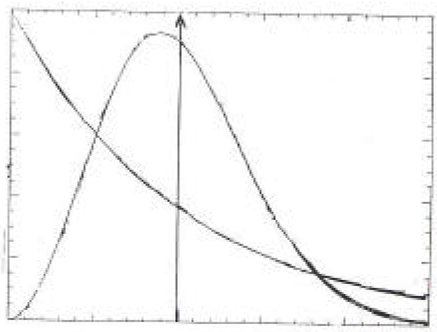

FIG. 4. Sketch of the TWD in terms of the normalized terrace width $s \equiv \lambda/\langle\lambda\rangle$ for the cases depicted in the preceding three figures.

Before closing, it is convenient for later nuggets in this series to introduce the idea of a step-step pair correlation function $h(s)$, which is the probability of finding a step at s, conditional on there being a step at the origin. It is generally easier to calculate this "2-particle" correlation function than the "many-particle" correlation function $P(s)$, for which there can be no step between the origin and s. Thus, for the perfect staircase of Fig. 1, $h(s)$ is obviously $\Sigma_n \delta(s - n)$. For the special case $A = 0$ of Fig. 3, $h(s)$ is just $1-[\sin(\pi s)/\pi s]^2$ [3], the pair correlation function of free fermions in one dimension. Later nuggets will discuss the source of this connection.

[1] M. E. Fisher and D. S. Fisher, *Phys. Rev. B* 25, 3192 (1982).

[2] B. Joós, T. L. Einstein, and N. C. Bartelt, *Phys. Rev. B* 43, 8153 (1991).

[3] M. L. Mehta, *Random Matrices*, 2^{nd} ed. (Academic, San Diego, 1991)