ELSEVIER

Applied Surface Science 175–176 (2001) 62–68

applied surface science

www.elsevier.nl/locate/apsusc

Terrace-width distributions on vicinal surfaces: generalized Wigner surmise and extraction of step–step repulsions

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Accepted 30 January 2001

Abstract

From quantitative measurement of the equilibrium terrace-width (ℓ) distribution (TWD) of vicinal surfaces, one can assess the strength A of elastic step–step repulsions A/ℓ^2. Generally the TWD depends only on $\tilde{A} = A \times (\text{step stiffness})/(k_B T)^2$. From ideas of fluctuation phenomena, TWDs should be describable by the ''generalized Wigner distribution'' (GWD), essentially a power-law in $\ell/\langle\ell\rangle$ times a ''Gaussian decay'' in $\ell/\langle\ell\rangle$. The power-law exponent is related simply to $\tilde{A}$. Alternatively, the GWD gives the exact solution for a mean-field approximation. The GWD provides at least as good a description of TWDs as the standard fit to a Gaussian (centered at $\langle\ell\rangle$). It works well for weak elastic repulsion strengths $\tilde{A}$ (where Gaussians fail), as illustrated explicitly for vicinal Pt(1 1 0). Application to vicinal copper surfaces confirms the viability of the GWD analysis. The GWD can be treated as a two-parameter fit by scaling ℓ using an adjustable characteristic width. With Monte Carlo and transfer-matrix calculations, we show that for physical values of $\tilde{A}$, the GWD provides a better overall estimate than the Gaussian models. We quantify how a GWD approaches a Gaussian for large $\tilde{A}$ and present a convenient, accurate expression relating the variance of the TWD to $\tilde{A}$. We describe how discreteness of terrace widths impacts the standard continuum analysis.

PACS: 05.40.+j; 61.16.Ch; 68.35.Md; 68.35.Bs

Keywords: Equilibrium thermodynamics and statistical; Mechanics; Surface structure; Morphology; Roughness; Topography; Stepped single crystal surfaces; Vicinal single crystal surfaces

1. Introduction

About a decade ago quantitative measurement of the widths ℓ of terraces on vicinal surfaces became feasible. The primary motivation for examining the terrace width distribution (TWD) is, arguably, that it provides the optimal way to assess the strength of the elastic (and/or dipolar) repulsion between steps. Building on ideas from three decades ago [1], contemporaneous theoretical work at Maryland was important in these early investigations of this problem [2]. Prompted by concerns raised by groups at Saclay [3–5] and at Grenoble [6,7], there has been renewed activity at Maryland on this subject [8–12]. Most

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0169-4332/01/$ – see front matter
PII: S0169-4332(01)00159-3

notably, we have recognized that since steps on vicinal surfaces should share general features of fluctuating systems, the TWD should exhibit certain universal properties. The goals of this short paper are to present a brief summary of this work, with a few new remarks, along with references for readers seeking more information. In particular, the first author recently presented an invited talk on the subject at the International Symposium on Surface and Interface — Properties of Different Symmetry Crossing — 2000 in Nagoya; readers are referred to the proceedings for a succinct review of the work [13].

Standard analysis procedures of TWDs make a continuum approximation in the direction along the steps, called $\hat{y}$ in "Maryland notation." (The perpendicular direction in the terrace plane, in the "downstairs" direction, then becomes $\hat{x}$.) In the highly successful [14] step continuum approach to vicinal surfaces, equilibrium properties are described in terms of two parameters: the step stiffness $\tilde{\beta}$ and some measure of the interaction strength. The former is essentially the thermal energy divided by the diffusivity, (the proportionality coefficient associated with the linear growth of mean-square wandering of steps in $\hat{x}$ with increasing y, starting from some position on the step). Generically, the interaction between steps consists of an elastic repulsion per length A/ℓ^2 and a temperature-dependent "entropic" repulsion — also $\propto \ell^{-2}$ — arising from the physical restriction that steps cannot cross each other. The repulsion is usually characterized by A. (It can also be characterized by a combination of the two. Note that this is not a simple sum, since as A increases, neighboring steps encounter each other less often, decreasing the entropic contribution.) In the ensuing description of TWDs, i.e. the fluctuations of ℓ from the average value $\langle\ell\rangle$, A appears only in the form of a *dimensionless interaction strength*

$$\tilde{A} \equiv A\tilde{\beta}(k_B T)^{-2} \tag{1}$$

Our guiding philosophy can be capsulized:

- The "standard analysis procedure" noted above is part of the step continuum approximation. In this perspective [14], the mesoscopic behavior of the step is characterized in terms of three parameters: and a parameter representing the dominant kinetics (a kinetic coefficient or diffusion constant times carrier density). Hence, a knowledge of $\tilde{A}$ is crucial to a proper description.
- In this approximation, because step overhangs are physically forbidden, the set of step configurations in 2D space maps into the world lines describing the evolution of non-crossing particles (spinless fermions or hard bosons) in 1D space. This mapping is what leads to most of the progress in theoretical understanding.
- In experiments to date, investigators have measured the distribution of terrace widths ℓ. This correlation function in essence is a many-particle correlation function, since one measures the probability of finding a pair particles separated by ℓ *with none between them.*

In experimental systems $\tilde{A}$ is typically between 0 and 15 [9,10,14] (cf., esp., Table 2 of Ref. [13]). When $\tilde{A}$ is not too small, the shape of a TWD can be adequately described by a Gaussian. However, as noted initially, there are conflicting theories on how to estimate $\tilde{A}$ from the variance of this Gaussian [1–7]. More recently, we have recognized [8–11] that the TWD might better be described using a simple expression arising from random-matrix theory, called the "generalized Wigner surmise." The underlying model [15,16] is exactly solvable only for $\tilde{A} = 0$ and $\tilde{A} = 2$ [17,18], as well as in the limit $\tilde{A} \to \infty$. Hence, to assess the merits of various approaches for general $\tilde{A}$, we had to generate well-characterized distributions numerically.

2. Fundamental results

2.1. Gaussian approximations to TWDs

For convenience and simplicity we initially divide ℓ by its average value $\langle\ell\rangle$, thus constructing the dimensionless parameter $s \equiv \ell/\langle\ell\rangle$. Then the TWD, $P(s)$, is not just normalized but has unit mean. The Gaussian approximation to the TWD takes the form

$$P(s) \approx P_G(s) \equiv \frac{1}{\sigma_G\sqrt{2\pi}} \exp\left[-\frac{(s-1)^2}{2\sigma_G^2}\right] \tag{2}$$

In addition to their simplicity and familiarity, Gaussians can be justified readily for strong elastic

repulsion between steps. In this limit the motion of each step is confined near its mean position; a Gruber–Mullins (GM) argument (in which a single step is treated as active and its two neighbors are fixed at twice $\langle \ell \rangle$) shows that [1,2]

$$\sigma^2 = K\tilde{A}^{-1/2} \tag{3}$$

For the GM case, with interactions only between nearest-neighbor steps, K is $1/\sqrt{48} \approx 0.144$. If all steps interact with A/ℓ^2, then the effective interaction increases by a factor of $\frac{1}{90}\pi^4 \approx 1.08^+$, decreasing the variance, and so K, by just 3^+ (to 0.139).

The Grenoble group [6,7] argued that the GM-derived variance underestimates (for given $\tilde{A}$) the true variance. For very large $\tilde{A}$ the entropy of interaction between steps becomes negligible (since the repulsions prevent their coming close together), so that the only entropy is that of the individual steps. Then, assuming *both* steps bounding a terrace fluctuate independently, the variance of the TWD should be the *sum* of the variances of the fluctuations of each step, i.e. *twice* the variance obtained in the GM picture (in which there is a *single* "active" step between a pair of fixed straight neighboring steps). Due to anticorrelations, σ^2 and so K increase by 1.801 (for given $\tilde{A}$) rather than doubling.

Including entropic repulsions in an average way [8] amounts to replacing $\tilde{A}$ by Eq. (3) by an effective interaction strength $\tilde{A}_{\text{eff}}$ obtained from the cubic term of the expansion of the projected free-energy of a vicinal surface as a function of misorientation slope [19]. The resulting enhancement is

$$\frac{\tilde{A}_{\text{eff}}}{\tilde{A}} \equiv \tfrac{1}{4}\tilde{A}^{-1}\left(\sqrt{4\tilde{A}+1}+1\right)^2 \sim 1 + \tilde{A}^{-1/2} + \tfrac{1}{2}\tilde{A}^{-1} + \cdots \tag{4}$$

This modification (which vanishes as $\tilde{A} \to \infty$) extends to smaller $\tilde{A}$ the range of viability of this (modified) asymptotic limit. In this approximation, including interactions with all steps decreases σ^2 and so K by nearly 10%. The Saclay group [3–5], alternatively, makes a continuum approximation in the $\hat{x}$-direction as well as $\hat{y}$ and invokes correlation functions from roughening theory to obtain a result of the form of Eq. (3), again with $\tilde{A}_{\text{eff}}$ replacing $\tilde{A}$, in which $K = 2/\pi^2 \approx 0.203$.

Since the various Gaussian approaches make different fundamental approximations, the detailed relationships between the width of the Gaussian and $\tilde{A}$ differ notably. Even when a TWD can be well fit by a Gaussian, the estimation of $\tilde{A}$ can be ambiguous.

2.2. Symmetry and Wigner approximation to TWDs: CGWD

Wigner long ago proposed that fluctuations in the spacings of energy levels of a system (originally nuclei) should exhibit certain universal features depending only on the symmetry — orthogonal, unitary, or symplectic — of the underlying couplings. This insight, promulgated using random-matrix theory [17,18], has been widely applied to fluctuation phenomena in chaotic systems. The pathway to this valuable information is the description of the equilibrium fluctuations of steps using the Calogero [15] and Sutherland [16] models of spinless fermions in 1D, interacting with a repulsion decaying as the inverse square of separation. Remarkably, the TWD becomes equivalent to the distribution of the energy spacings, which can be solved exactly by random-matrix methods for the three symmetries. According to the so-called Wigner surmise, these exact solutions for the three distribution of fluctuations can be approximated by [20]

$$P_\varrho(s) = a_\varrho s^\varrho \exp(-b_\varrho s^2) \tag{5}$$

where the constants b_ϱ associated with unit mean of $P(s)$ and a_ϱ deriving from normalization are

$$b_\varrho = \left[\frac{\frac{1}{2}\Gamma\left(\frac{\varrho+2}{2}\right)}{\frac{1}{2}\Gamma\left(\frac{\varrho+1}{2}\right)}\right]^2 \quad \text{and} \quad a_\varrho = \frac{2b_\varrho^{(\varrho+1)/2}}{\Gamma\left(\frac{\varrho+1}{2}\right)} \tag{6}$$

The variance of $P_\varrho(s)$ is

$$\sigma_{\text{W}}^2 = \frac{\varrho+1}{2b_\varrho} - 1 \underset{\varrho\to\infty}{\sim} \frac{1}{2\varrho} \tag{7}$$

The three symmetries correspond to the values $\varrho = 1$, 2, or 4, respectively. This trio of expressions are outstanding approximations, accurate to better than ± 0.004 for the latter two cases (cf., esp., Fig. 4.2a of Ref. [20]). From the mapping of the step problem onto the Sutherland [16] Hamiltonian comes the relation

$$\tilde{A} = \tfrac{1}{4}\varrho(\varrho-2) \tag{8}$$

Inverting Eq. (8) gives $\varrho = 2\sqrt{\tilde{A}_{\text{eff}}}$ (cf. Eq. (4))!

The three special values of ϱ correspond to $\tilde{A} = -\frac{1}{4}$, 0, or 2, respectively. The second case describes steps interacting only via the entropic repulsion, while the first indicates a physically unlikely attraction. The third case, $\tilde{A} = 2$, corresponds to a rather moderate repulsion. As documented in Table 1 of Refs. [8,13], the variance of Wigner's $P_\varrho(s)$ is nearly the same as the exact value. The Saclay and GM estimates are a few percent too low, while the modified Grenoble estimate is much too high.

The crucial question is how to generalize to other values of $\tilde{A}$. We simply use Eq. (5) for *arbitrary* value of $\varrho \geq 2$, with ϱ related to $\tilde{A}$ by Eq. (8). This distribution, for general ϱ, is denoted the CGWD (continuum generalized Wigner distribution). While there are no symmetry arguments to justify the CGWD form, there are arguments in its favor:

- $P_\varrho(s)$ should give a decent approximation of the TWD for values of ϱ between 2 and 4 since the range in parameter space is small. In any case, the Gaussian approximations are invalid in this regime.
- For very large $\tilde{A}$, the Grenoble viewpoint becomes compelling. In this limit, the leading term in the expansion of σ^2_W in Eq. (7) implies that $K_W = \frac{1}{4}$ in Eq. (3), with $\tilde{A}_{\text{eff}}$ replacing $\tilde{A}$. Thus, as listed in Table 1, the CGWD variance approaches the (modified) Grenoble estimate nicely, while the Saclay estimate is notably too small. Since the CGWD does well for both $\varrho \to \infty$ and $\varrho = 4$, it is a promising candidate for intermediate values.
- As a function of s, the CGWD not only has the Gaussian behavior expected (from random-walker analogies) at large s but also reproduces the exact power of s for $s \ll 1$. In this limit, the many-step correlation function becomes identical to the pair correlation function, which $\propto s^\varrho$, with a prefactor similar to a_ϱ [21–25].
- We can derive the CGWD from a Schrödinger-equation approach [11], as discussed below.

To test numerically the accuracy of Eq. (5) we apply standard Monte Carlo methods to the simplest adequate model, the terrace-step-kink (TSK) model. The only thermal excitations are kinks of energy ϵ along the steps. For simplicity we consider a vicinal simple cubic lattice with unit lattice constant. The stiffness $\tilde{\beta}_{\text{TSK}}$ of an isolated step — needed to extract A from $\tilde{A}$ — is then simply $2k_BT \sin h^2(\epsilon/2k_BT)$ [26]. This model is obviously *discrete* in the $\hat{y}$ as well as the $\hat{x}$ directions [2,3,5,26].

In Fig. 2 of Ref. [13] we provide some preliminary results for the case $\langle \ell \rangle = 6$ at $k_BT/\epsilon = 0.5$, with $L_y = 200$ and the number of steps $N = 10$. In addition to the standard Metropolis algorithm [27], we use the "refusal-free" n-fold way [28,29], especially for large $\tilde{A}$ (or at low T), where it is much more efficient than the Metropolis algorithm. The elastic repulsion is here considered only between neighboring steps, a common simplification in Monte Carlo [2,4]. The key result is that the CGWD provides globally the best accounting of the variance as a function of $\tilde{A}$.

3. Useful results for interpreting experiments

We here collect some useful formulas and ideas derived earlier (mostly in Ref. [10]). From Eq. (8) and series expansions comes the arguably optimal expression from which to estimate $\tilde{A}$ from σ^2:

$$\tilde{A} \approx \tfrac{1}{16}[(\sigma^2)^{-2} - 7(\sigma^2)^{-1} + \tfrac{27}{4} + \tfrac{35}{6}\sigma^2] \tag{9}$$

with all four terms needed to provide a good approximation over the full physical range of $\tilde{A}$. As in Eq. (3) the Gaussian methods essentially use just the first term of this expression and adjust the prefactor. For large enough (see Ref. [10]) $\tilde{A}$, those preferring Gaussians over $P_\varrho(s)$ of Eq. (5) can extract σ^2 from their fit and then apply Eq. (9).

When fitting experimental data, it is often fruitful to generalize the CGWD to a two-parameter fit. The central idea is that the characteristic length by which ℓ is normalized should be taken as an adjustable parameter $\overline{\ell}$ rather than as the first moment $\langle \ell \rangle$, as it would be ideally. Normalized data are then fit to

$$\left(\frac{\langle \ell \rangle}{\overline{\ell}}\right) P_\varrho\left(\frac{\ell}{\overline{\ell}}\right) \tag{10}$$

In the experimental systems studied to date, $\langle \ell \rangle / \overline{\ell}$ tends to be greater than unity, typically by several percent. In contrast, our companion Monte Carlo simulations [12] find that the optimal $\overline{\ell}$ is essentially identical to $\langle \ell \rangle$.

In a careful study of the effects of lattice discreteness in the $\hat{y}$ direction, we found two major results [10]. (1) When $\langle \ell \rangle \geq 4, \tilde{A}$ using the CGWD provides a

satisfactory estimate over the range of physically reasonable dimensionless repulsions. (2) As the TWD becomes narrower at large $\tilde{A}$, using the CGWD to estimate $\tilde{A}$ becomes questionable. This breakdown occurs for ϱ near $\langle\ell\rangle^2$, i.e. when the squared interstep spacing becomes comparable to the variance. Analogous problems at high misorientation also occur when continuous Gaussians are used as the fitting functions.

To estimate uncertainties in the determination of the TWD and, ultimately, $\tilde{A}$, one needs a good estimate of the number of *independent* measurements, which is generally much smaller than the total number of measurements. This issue is treated in Ref. [10], where a rough calculation shows that the reduction factor can be nearly two orders of magnitude, emphasizing the need for using several STM images to obtain decent statistics.

4. Applications to experimental TWDs

In two papers [9,10], we applied these ideas to extensive data on Cu {1 0 0} and {1 1 1} vicinals, each at three different misorientations, and these six cases at various temperatures. In all, around 30 different cases were considered. Several trends appeared: the value of $\overline{\ell}$ derived from the two-parameter fit to a CGWD is almost always smaller than $\langle\ell\rangle$ given by the mean of the TWD. The directly measured variances usually exceed the values deduced from any of the fitted curves (cf. Section 7 of Ref. [10]). The value of ϱ deduced from the two-parameter CGWD fit is higher than that from the single-parameter version, and the resulting σ^2 is typically closer to that deduced from the Gaussian fit. For ''good'' data — in which the measured TWD behaves essentially monotonically on either side of the peak — $\overline{\ell}/\langle\ell\rangle$ differs from unity by a few percent, and the change in ϱ and σ^2 is negligible. When the TWD has a double-peak or hump at large s, $\overline{\ell}/\langle\ell\rangle$ is at least twice as far below unity, and the two-parameter-fit curve is narrower than the single-parameter-fit curve.

We also studied data for vicinal Pt(1 1 0) at room temperature; the terraces are (1×2) reconstructed, with ''(1×3)''-segment steps. Recent measurements show that the interaction between their steps is small [30], rendering traditional Gaussian approximations invalid. Fits to the CGWD yield $\varrho = 2.06$ ($\tilde{A} = 0.0309$) or, when done in the two-parameter way, $\varrho = 2.24$ ($\tilde{A} = 0.134$) [10]; in the latter case, the optimal $\overline{\ell}/\langle\ell\rangle$ is 91% and the fit is notably better. The presence of a high-s bulge indicates this feature is not peculiar to the vicinal Cu systems of [9,10].

5. New directions

In addition to measuring TWDs, experimentalists should be able to obtain the distributions of the distances between pairs of steps having n steps, $n = 1, 2$, or more, between them. This supplementary data could provide a valuable consistency check. For the three special cases $\varrho = 1, 2, 4$, these distributions have recently been investigated theoretically in a different context [31]; the main assumption is that the conditional probability density of occurrence of a step at a given distance from a fixed step, with n steps in between, can be expressed in terms of the $(n+1)$th power of the corresponding probability for this distance with no intermediate steps. The generalization is discussed in Ref. [13]. Preliminary Monte Carlo checks find good agreement with the prediction for the double-terrace-width $(n = 1)$ case, but just adequate agreement for the case $n = 2$. Alternatively, one can simply measure the step–step correlation function, regardless of the number of intermediate steps. The advantage is that there are analytic results available [22], which we are in the process of applying to data.

Since a formal symmetry-derived basis of the CGWD exists only for the three special values of ϱ, we have developed arguments using Schrödinger equations to find circumstances under which it can be justified for arbitrary-strength repulsions [11]. The formalism also allows treatment of more general potentials than the inverse-square term characterizing the long-range behavior of elastic interactions. Of particular physical importance are the higher-order terms that enter at smaller terrace widths and an oscillatory interaction mediated by electronic surface states [32], expected [33] to have the form

$$\ell^{-2}\cos(2k_F\ell + \phi), \tag{11}$$

where k_F is the wavevector of the surface state at the Fermi level and ϕ is a phase shift associated with scattering from the pair of steps.

A wave function $\psi_0(s)$ defined such that $\psi_0^2 \equiv P_\varrho(s)$ satisfies the Schrödinger-like equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}s^2}\psi_0(s) + [\tilde{A}s^{-2} - b_\varrho(\varrho+1) + b_\varrho^2 s^2]\psi_0(s) = 0 \tag{12}$$

The new potential term $\tilde{U}(s) = b_\varrho^2 s^2$ is a dimensionless projected free-energy representing interactions with all the other steps not explicitly considered in the dimensionless step interaction $\tilde{A}s^{-2}$, while $b_\varrho(\varrho+1)$ is the eigenvalue of the ground state. In this framework, by substituting more general potentials for $\tilde{A}s^{-2}$ in Eq. (12) and solving for the ground-state wavefunction, we can contend analytically with more complicated potentials. Successful tests are described in Ref. [11]. Though tempting, it is dangerous to invert straightforwardly the preceding approach to deduce the underlying interaction potential from the experimental TWD. We have devised a more successful, albeit laborious, procedure to do so [11].

6. Closing summation

The CGWD, expressed in Eq. (5), provides an excellent interpolation between the exactly solvable cases at $\tilde{A} = 0$ and $\tilde{A} = 2$, and approaches the correct limit for very large $\tilde{A}$. It gives the qualitative behavior of variance as a function of $\tilde{A}$, and numerical evidence suggests that it interpolates well when $\tilde{A}$ is large. The TWDs shape approaches a Gaussian in this regime of moderately strong $\tilde{A}$; the CGWD (via Eq. (9)) then offers the best estimate of $\tilde{A}$ from the variance. As is evident from Eq. (3), any fractional error in gauging the width or variance of the TWD is greatly amplified when subsequently estimating $\tilde{A}$. When there are active surface states near the Fermi energy, the TWD should exhibit notable deviations from a CGWD (or a Gaussian).

The theory of random fluctuations in complex systems has concentrated on the three special values of ϱ (with some attention to intermediate values), i.e. the range of $\tilde{A}$ weaker than in most physical systems. Further effort is warrant to probe why the CGWD works so well when there is no fundamental symmetry argument to justify it. The step–step pair correlation function, which can be analyzed in greater detail theoretically than the TWD, can be measured almost as easily as it. Multistep correlations should also not be neglected in experiments measuring TWDs.

Acknowledgements

Work was supported by the NSF-MRSEC at University of Maryland, done in collaboration with N.C. Bartelt, B. Joós, E.D. Williams, J.E. Reutt-Robey, et al. at UM, and with M. Giesen and H. Ibach at FZ-Jülich (via a Humboldt US Senior Scientist Award). SDC participated in an NSF-MRSEC-sponsored REU program.

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