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Terrace width distributions for vicinal surfaces with steps of alternating stiffness

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Abstract

For the typical elastic interactions between steps, the generalized Wigner distribution (GWD) has been shown to be in excellent quantitative agreement with terrace width distributions (TWDs) calculated from numerical simulations. Here we show that the TWDs of vicinal surfaces with steps of alternating stiffness (but the same sort of step–step repulsions) are also given by the GWD. In the key parameter, the dimensionless repulsion strength, the step stiffness is generalized to twice the "reduced stiffness" of the two kinds of steps, as befits the inertial nature of stiffness. These results should also be applicable to more general surfaces with steps of different stiffness.

Keywords: Equilibrium thermodynamics and statistical mechanics; Stepped single crystal surfaces; Surface structure, morphology, roughness and topography; Surface energy; Vicinal single crystal surfaces

1. Introduction

When a crystal is cleaved at a small angle to a high-symmetry direction (corresponding to small Miller indices), the newly exposed surface is often composed of terraces of the high-symmetry surface separated by steps of one or a few atoms in height [1]. The lower coordination number of surface atoms can lead to relaxations [1–9], in atomic position, reconstruction [1,2,7,10–13] of the surface into a different order, and the creation of new electronic states not present in the bulk material [14,15]. Such a vicinal, or stepped, surface can be exploited for use in catalysts [10,11,16], or for growing structures such as quantum wires and other electronic components [17], as well as for basic scientific research.

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The relaxations, reconstructions, and surface electronic states give rise to effective interactions between steps, which obviously can be quite complicated in general. In most cases, though, the interactions between two neighboring steps are believed to be approximately described by the potential [1,13,18].

$$V(L) = \frac{A}{L^2}, \tag{1}$$

where A is an interaction constant and L is the width of the terrace (see Fig. 1). This potential is the dominant term in an expansion of the elastic interactions, and Eq. (1) is considered by most researchers in the field to sufficiently describe all step–step interactions.

Although the interaction between steps has been calculated for a few model surfaces, the elastic interactions require large numbers of atoms to be included in the calculations, which makes them computationally demanding. (See, e.g, Refs. [8,9].) Furthermore, the results are somewhat dependent on approximations used to simplify the quantum-mechanical treatment of electrons. A more practical method for determining fundamental parameters, such as the interaction constant A and the kink energy ε, is to infer them from experimental measurements of statistical properties, such as the terrace width distribution [19,20] (TWD) and

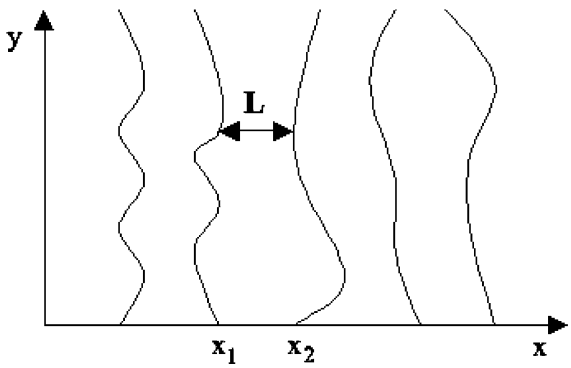

Fig. 1. Steps can be mapped onto the world-lines of spinless fermions. The average direction of the steps (y in "Maryland notation") maps onto (imaginary) time. L is the width of the terrace between the steps at x_1 and x_2.

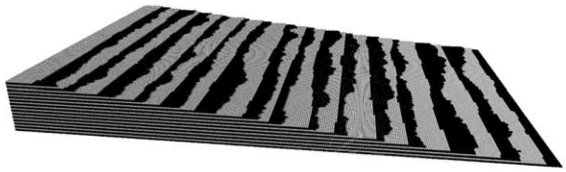

Fig. 2. TSK model of an AB-type vicinal crystal surface. The stiffness of steps with light terraces to the left is greater than the stiffness of the steps with dark terraces to the left. In this illustration, there is no interaction between the steps ($\tilde{A} = 0$), and the stiffness ratio is $R = 8$.

wandering function [19,21], $\langle [x_i(y + \Delta y) - x_i(y)]^2 \rangle$, which is related to spatial autocorrelations.

The organization of this paper is as follows [22]. In Section 2 we review some approximations for TWDs for vicinal surfaces with steps all of the same stiffness. In Section 3, we extend the discussion of Section 2 to cover the case in which the steps do not all have the same stiffness, with particular attention to the case in which two types of steps alternate (Fig. 2). Silicon surfaces vicinal to the (1 0 0) plane are perhaps the most important example of such surfaces. (For a review of stepped Si surfaces, see Ref. [23].) Another realization is a surface vicinal to the basal plane of an hcp crystal in a principal direction such that the step edges are close-packed. A vicinal surface with metallic decoration on the lower side of each step, as for [wide] quantum wires, could also exhibit such properties, In this first attack on the problem, we neglect the possibility that the alternating stiffnesses may well be associated with alternating stress domains that can lead to more complicated interactions between steps [24]. Section 4 shows that TWDs derived from Monte-Carlos simulations of the Terrace-Step-Kink (TSK) model are in agreement with the predictions of Section 3. We summarize and conclude with a discussion of the relevance of this work to more complicated systems, such as vicinal surfaces of superlattices, in Section 5.

2. Approximate hamiltonians and terrace width distributions

When the step–step interactions are described by Eq. (1), the static properties of a system of