Available online at www.sciencedirect.com
ScienceDirect
Surface Science 601 (2007) 3979–3983
SURFACE SCIENCE
www.elsevier.com/locate/susc

Facet-edge fluctuations with periphery diffusion kinetics

M. Degawa [a], T.J. Stasevich [a], A. Pimpinelli [b], T.L. Einstein [a], E.D. Williams [a,*]

[a] Department of Physics, Materials Research Science and Engineering Center, University of Maryland, College Park, MD 20742-4111, USA
[b] LASMEA, UMR 6602 CNRS, Université Blaise Pascal, Clermont 2, F-63177 Aubière Cedex, France

Available online 21 April 2007

Abstract

We investigate the novel scaling of the steps bounding a facet surrounded by a rough region. The hindered, asymmetric fluctuations can be associated with the emergence of a dominant non-linear term in the Hamiltonian governing the step fluctuations. We explore the crossover from unhindered to hindered fluctuations, calculating the growth exponent, β, with Monte Carlo simulation within the TSK model. The hindered behavior is found in the simulations when the facet-edge step is separated by fewer than six atomic spacings from the second step. Actual fluctuations are larger than in this calculation, particularly at higher temperatures, making the hindered behavior easier to observe. In addition, we discuss the possibility that volume conservation effects in nanoscale structures may cause similar confinement in non-conserved fluctuations.

Keywords: Equilibrium thermodynamics and statistical mechanics; Terrace-step-kink model; Monte Carlo simulations; Surface diffusion; Surface (step) tension; Kinks; Steps; Adatoms

1. Introduction

Due to the rapid growth of interest in quantum computing and the related demand for creating quantum dots, controlled fabrication of nano-structures has become of great importance [1–4]. For the evolution of nano-structure, the control of step dynamics is crucial, since the steps are the fundamental building blocks of crystalline surfaces. The equations of motion for straight steps on a vicinal surface are well understood within the continuum step model e.g. as applied to MBE growth and step bunching. The power of this model is that it can be applied to both analysis of experimental observations [5–8] and comparison to microscopic models, such as the terrace-step-kink (TSK) model, using statistical methods and a handful of key parameters [6,9]. In particular, Langevin-type analysis of the statistical properties of steps can be used to relate the physical properties of isolated steps to the thermodynamic parameters of the continuum step model. Application of the Langevin approach has shown that the experimentally accessible correlation functions (defined below) scale as $\sim y^{2\alpha}$ and $t^{2\beta}$, where α and β are the roughness and growth exponents, respectively. For isolated steps, $\alpha = 1/2$, characteristic of a random walk, and β depends on the principal mass transport mechanism, e.g. attachment–detachment (A/D), $\beta = 1/4$, and periphery diffusion (PD), $\beta = 1/8$ [5,6].

However, for nano-structures, the step equations of motion are not obvious due to the finite volume effects of the nano-structure [10,11]. Although the steps can still be viewed as 1D interfaces, not only local deformations but global effects (overall shape and mass conservation) must be considered to obtain the equations of motion. In a previous paper [12], we showed that a global curvature of an island or a step at a facet-edge, as illustrated in Fig. 1a and b, alters the step chemical potential compared to an isolated step by breaking the symmetry of adatom motion to the upper and lower terrace, resulting in a non-linear equation of motion for the step. For a facet, furthermore, the suppression of the fluctuation amplitude due to the existence of a neighboring step alters the scaling behavior of the noise term in the Langevin equation. Such changes lead to two different university classes of dynamic scaling,

* Corresponding author. Tel.: +1 301 405 6156; fax: +1 301 314 9465.
E-mail address: edw@physics.umd.edu (E.D. Williams).

0039-6028/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.susc.2007.04.097

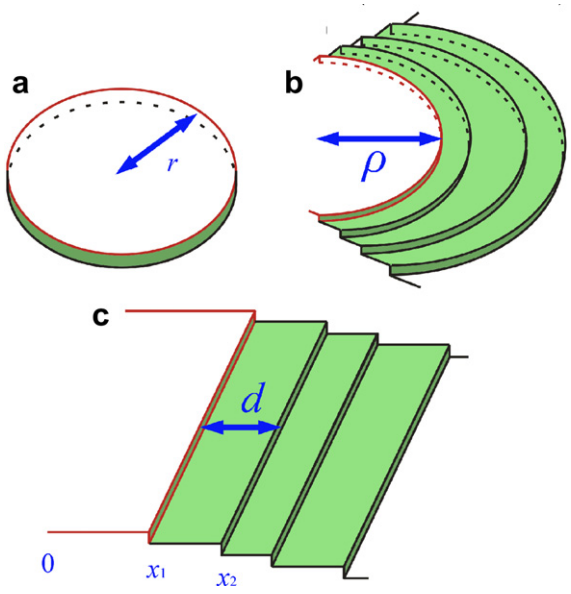

Fig. 1. Schematic drawing of the continuum step model in the three cases of (a) an island with radius r (b) a facet of a finite volume crystallite (with curvature) with radius ρ and (c) a facet of a infinite volume crystallite (straight steps) with $d = x_2 - x_1$.

with $\alpha = 1/3$ [13] for both and $\beta = 1/5$ and $\beta = 1/11$ for A/D and PD, respectively [12].

Another previous conclusion [12] was that the global curvature effect will be important for an island only when its circumference is small compared to the capillary length; this translates to a very severe condition on the equilibrium chemical potential of the island ($\mu_{eq} > 2\pi\beta\tilde{\beta}\Omega/k_BT$) [14,15]. In this paper, we show with the use of the continuum step model that even with no curvature (straight steps), a facet-edge step interacting with a single fixed neighboring step, with dynamics conserving mass, can have a non-linear term in the equation of motion. Monte Carlo simulations using the TSK model are performed to confirm the proposed effects.

2. Background

The continuum step model uses a discrete array of 1D continuous interfaces to represent the steps on the surface. A facet-edge step of a crystallite with infinite volume (straight steps) is illustrated in Fig. 1c. With appropriate approximations, the step equation of motion is given by a Langevin equation

$$\frac{\partial x(y,t)}{\partial t} = f[x(y,t)] + \eta(y,t), \tag{1}$$

where $x(y,t)$ is the position of the facet-edge at time t, $f[\bullet]$ is a function of $x(y,t)$ describing the deterministic relaxation process, and $\eta(y,t)$ is a noise term, which can be conservative or non-conservative depending on the nature of $f[\bullet]$. The free energy of the facet step with a projected length L is

$$F = \int_0^L \left(\beta(\theta)\sqrt{1 + \left(\frac{\partial x}{\partial y}\right)^2} + \frac{gh^3}{(x_2 - x)^2} \right) \mathrm{d}y, \tag{2}$$

where β is the step free energy per length, g is the step interaction coefficient, h is the step height and x_2 is the position of the neighboring step, which is approximated as straight and fixed in position. The step chemical potential is derived as

$$\mu[x,\dot{x},\ddot{x}] = \frac{\delta F}{\delta N} = \Omega\left(\frac{-\tilde{\beta}\ddot{x}}{\sqrt{(1+\dot{x}^2)^3}} + \frac{2gh^3}{(x_2 - x)^3} \right), \tag{3}$$

where Ω is the atomic area, $\tilde{\beta} = \beta + \partial^2\beta/\partial\theta^2$ is the step stiffness, and the superscript dot denotes differentiation with respect to y. The deterministic part of the Langevin equation is obtained by modeling the microscopic transfer processes at the facet step-edge. Non-conserved dynamics is used to represent the random A/D of adatoms from the reservoir as

$$\frac{\partial x(y,t)}{\partial t} = \frac{-\Gamma_{AD}}{k_BT}\mu[x,\dot{x},\ddot{x}] + \eta(y,t), \tag{4}$$

where Γ_{AD} is the A/D-driven step mobility and $\eta(y,t)$ is non-conserved white noise. Similarly for PD, conserved dynamics is used to represent atoms moving along the step edge

$$\frac{\partial x(y,t)}{\partial t} = \frac{\Gamma_{PD}}{k_BT}\frac{\partial^2\mu[x,\dot{x},\ddot{x}]}{\partial y^2} + \eta_C(y,t), \tag{5}$$

where Γ_{PD} is the edge-hopping-driven step mobility (differing from Γ_h of Ref. [5] by a factor of Ω), and $\eta_C(y,t)$ is conserved white noise.

3. Results

To obtain the stable mean position x_1 of the facet-edge, Eq. (3) is set equal to the "reservoir" chemical potential μ_0 of the crystallite [11]. Neglecting the local curvature term (first term) in Eq. (3) gives

$$x_1 = x_2 - h\left(\frac{2\Omega g}{\mu_0}\right)^{1/3} \quad \text{or} \quad d = h\left(\frac{2\Omega g}{\mu_0}\right)^{1/3} \tag{6}$$

where $d = x_2 - x_1$ is the distance between the top two steps as shown in Fig. 1c. Assuming the fluctuations to be small, Eq. (3) is expanded about this x_1.

$$\mu[x,\ddot{x}] = -\Omega\tilde{\beta}\ddot{x} + \mu_0 + \frac{3}{h}\left(\frac{\mu_0^4}{2\Omega g}\right)^{\frac{1}{3}}(x - x_1) + \frac{3}{h^2}\left(\frac{2\mu_0^5}{\Omega^2 g^2}\right)^{\frac{1}{3}}(x - x_1)^2 + \cdots. \tag{7a}$$

Using dimensionless variables,

$$\tilde{x} = \frac{x - x_1}{d}, \quad \tilde{y} = \frac{y}{d}, \quad \tilde{\mu} = \frac{\mu d}{\Omega\tilde{\beta}}, \quad \tilde{g} = \frac{gh^3}{\tilde{\beta}d^2} \tag{7b}$$