Self-organization on surfaces/Auto-organisation sur les surfaces

Dynamics of crystal steps

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Available online 12 January 2005

Presented by Guy Laval

Abstract

In this article, we wish to point out some of the recent advances in the study of step dynamics on crystal surfaces. We will first list some approaches to steps dynamics, based on irreversible thermodynamics, kinetic roughening concepts, and mass transport mechanisms. In a second part, we shall analyze step motion coupled to the diffusion of mobile atoms on terraces. A special focus will be given on pattern formation on vicinal surfaces and two-dimensional islands. Finally, we will report on the consequences of elastic and electronic relaxation on the dynamics of steps and adatoms. *To cite this article: O. Pierre-Louis, C. R. Physique 6 (2005).*

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Résumé

Dynamique des marches atomiques. Nous présentons quelques avancées récentes dans l'étude de la dynamique des marches cristallines. Nous mentionnerons tout d'abord différentes approches pour la modélisation de la dynamique des marches, basées sur la thermodynamique des processus irréversibles, les théories de rugosification, et le transport de masse. Dans une deuxième partie, nous analyserons le mouvement de marches couplées à la diffusion des atomes mobiles à la surface. Nous développerons particulièrement le cas des surfaces vicinales et des îlots bidimensionnels. Finalement, nous étudierons les conséquences de la relaxation élastique et électronique du solide sur la dynamique des marches et des adatomes. *Pour citer cet article : O. Pierre-Louis, C. R. Physique 6 (2005).*

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1. What is a step?

1.1. Steps, terraces and adatoms

When one looks at a crystal at small scales during growth, the first surprising observation is that growth usually proceeds via the lateral flow of atomic steps (see Fig. 1). Rather than sticking to the crystal at the place where they have landed, atoms indeed diffuse until they attach to a step, thereby leading to the forward motion of steps. As reported in the work of Burton, Cabrera and Frank in 1951, the analysis of crystal growth can therefore be based on the analysis of step motion. Following this work,
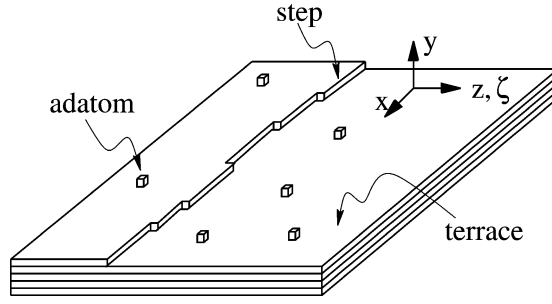
Fig. 1. Monoatomic crystal step, terrace, and adatom.

step motion has been widely studied to understand the formation of patterns at the nanometer and micrometer scales. In this review, we wish to present some of the recent advances in the analysis of step motion. More specifically, three questions will be our main focus: (i) What are the equations of motion and the structure of steps in non-equilibrium conditions, and at small scales? (ii) What are the patterns that are induced by step motion? (iii) What are the interactions between steps and atoms?

These three questions are the keys to the understanding of nanostructure formation, as a result of the nonlinear dynamics of fronts in non-equilibrium conditions, and involving long range interactions.

1.2. Buron–Cabrera–Frank model

Following the famous work of Burton Cabrera and Frank [1], we shall first model step kinetics in a macroscopic and phenomenological fashion, i.e. without referring to the underlying discreteness.

At the steps, mass conservation imposes:

$$\left(\frac{1}{\Omega} + c_- - c_+\right)V_n = -D\mathbf{n} \cdot \nabla c_- + D\mathbf{n} \cdot \nabla c_+, \tag{1}$$

where V_n is the normal step velocity, $\pm$ respectively denote the upper and lower sides of the steps, D is the diffusion of mobile atoms on terraces, c is their concentration, and Ω is the atomic area. On terraces (between the steps), we have, for example, during growth or sublimation:

$$\partial_t c = D\nabla^2 c + F - \frac{c}{\tau}, \tag{2}$$

where F is the incoming flux and τ is the typical adatom desorption time. The kinetic boundary conditions for the concentration in the vicinity of the steps are obtained by an assumption of linear kinetics, i.e. the diffusion mass flux arriving at the step is taken to be proportional to the departure from equilibrium at the step [2]:

$$D\mathbf{n} \cdot \nabla c_+ = \nu_+(c_+ - c_{eq}^*) + \nu_0(c_+ - c_-),$$
$$-D\mathbf{n} \cdot \nabla c_- = \nu_-(c_- - c_{eq}^*) + \nu_0(c_- - c_+), \tag{3}$$

where $\nu_\pm$ and ν_0 are attachment-detachment and transparency kinetic coefficients, the role of which will be discussed later. The local equilibrium concentration c_{eq}^* is computed from the Gibbs–Thomson relation,

$$c_{eq}^* = c_{eq} \exp(\mu/k_B T), \tag{4}$$

where c_{eq} is the reference equilibrium concentration. One has $\mu = \Omega\tilde{\gamma}\kappa$, where κ is the step curvature, and $\tilde{\gamma} = \gamma + \gamma''$ is the step stiffness, with γ the line tension of the step. When the radius of curvature of the step $1/\kappa$ is much larger than $\Gamma = \Omega\tilde{\gamma}/k_B T$, we may linearize Eq. (4), so that:

$$c_{eq}^* = c_{eq}(1 + \Gamma\kappa). \tag{5}$$

Additional contributions to μ coming for example from interactions between steps will be considered in the next sections.

Eqs. (1), (3) are not the only possible formulation of the boundary conditions. Indeed, linear combinations of the boundary conditions give rise to new formulations, some of which are listed in [3].

The kinetic coefficient ν_0 was introduced in [2], and accounts for 'direct' exchange between terraces: this phenomena is called step transparency, or step permeability. When steps are perfectly transparent $\nu_0 \to \infty$, the boundary conditions can be expressed as