# Step Bunching Induced by Drift of Adatoms with Anisotropic Surface Diffusion

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By means of Monte Calro simulation we study step bunching induced by the drift of adatoms with anisotropic surface diffusion. Like a vicinal face of Si(001), we suppose two types of terraces appear alternately, and their directions of fast diffusion are parallel and perpendicular to the steps. When the drift is perpendicular to the steps, we found from stability analysis that the vicinal face is unstable for pairing instability with both step-up and step-down drift. In a late stage of bunching, large bunches appear irrespective of the drift direction, while formation process of the bunches is affected by the drift direction.

## 1. Introduction

In a Si(001) vicinal face which is reconstructed to form dimer rows, two types of terraces of $1 \times 2$ and $2 \times 1$ structures appear alternately and steps act as domain boundaries. When a specimen is heated by direct electric current, a vicinal face is unstable [1] and large bunches appear irrespective of the current direction [2, 3]. The type of large terraces between the bunches, however, changes: the $1 \times 2$ terraces appear with the step-down current and the $2 \times 1$ terraces with the step-up current.

Stability of a Si(001) vicinal face has been studied by using a one-dimensional discrete step model [4]. The cause of instability is considered to be the drift of adatoms induced by the direct electric current. When the anisotropy of surface diffusion coefficient is taken into account, pairing of steps occurs irrespective of drift direction. The type of terraces between the step pairs is determined by the drift direction. The terrace with fast diffusion perpendicular to the step appears with the step-up drift, while the terrace with fast diffusion parallel to the step appears with the step-down drift.

Behavior of steps after the pairing of steps has been studied by Natori and co-workers with a numerical simulation of the one-dimensional step model with step repulsion [5, 6]. With the step-up drift large bunches appear by coalescence of step pairs. With the step-down drift the vicinal face is stable when the step distance is sufficiently small. If the step distance is large, the step pairing occurs, but large bunches do not appear, which does not agree with the experiments [2, 3].

In those theoretical analyses steps are assumed impermeable for over-step diffusion of adatoms. Step permeability is known to affect the condition to induce step bunching and wandering with isotropic surface diffusion [7, 8]. In this paper, by carrying out a Monte Calro simulation, we study the drift-induced bunching instability of permeable steps with the anisotropic surface diffusion. We show that the bunches are formed irrespective of the drift direction in agreement with experiment.

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## 2. Model for Monte Calro simulation

We use a square lattice model with the lattice constant (and the step height) $a = 1$. $x$-axis is parallel to the steps and $y$-axis is in the step-down direction. Boundary conditions are periodic in the $x$-direction and helical in the $y$-direction. We forbid two-dimensional nucleation and use solid-on-solid steps, i.e. the step position is a single-valued function of $x$. We neglect long range step-step interaction, but forbid overlapping of steps. There is no impingement and no evaporation of adatoms.

We consider two types of terraces. In one terrace, which we call terrace A, the surface diffusion is fast in the $y$-direction, and in the other terrace, which we call terrace B, the surface diffusion is fast in the $x$-direction. We choose the time increment for a diffusion trial such a way to make the surface diffusion coefficient for the fast diffusion $D_{\mathrm{s}} = 1$. We assume that the drift of adatoms is in the $y$-direction. In the terrace B, an adatom on the site $(i, j)$ moves to $(i \pm 1, j)$ with the probability $1/4$ and to $(i, j \pm 1)$ with the probability $p(1 \pm Fa/2k_{\mathrm{B}}T)/4$, where $p$ and $F$ represent the anisotropy of the surface diffusion and the external force that induces the drift. In the terrace A, an adatom on the site $(i, j)$ moves to $(i \pm 1, j)$ with the probability $p/4$ and to $(i, j \pm 1)$ with $(1 \pm Fa/2k_{\mathrm{B}}T)/4$. We assume two types of terraces appear alternately and the steps are permeable [7–9]. The diffusion between neighboring terraces occurs with the transition probability of the upper side terrace.

When an adatom comes in front of a step, solidification of the adatom occurs with the probability [8]

$$p_{\mathrm{s}} = \left[1 + \exp\left(\frac{\Delta E_{\mathrm{s}} - \phi}{k_{\mathrm{B}}T}\right)\right], \tag{1}$$

where $\Delta E_{\mathrm{s}}$ is the increment of the step energy and $\phi$ the chemical potential gain by the solidification. When there is no adatom on the top of a step atom, melting of the atom occurs with the probability

$$p_{\mathrm{m}} = \left[1 + \exp\left(\frac{\Delta E_{\mathrm{s}} + \phi}{k_{\mathrm{B}}T}\right)\right]^{-1}. \tag{2}$$

## 3. Result of simulation

In our simulation the system size is $128 \times 128$, the step number is 32, $p = 1/2$ and $Fa/k_{\mathrm{B}}T = \pm 0.3$ ($+(-)$ indicates the step-down (step-up) direction). Figure 1 represents snap shots of the step bunching. The upper (smaller $y$) side terrace of a solid line is the terrace A and that of a dotted line is the terrace B. Pairing of steps occurs irrespective of the drift direction((a) and (b)). The type of the large terrace separating step pairs changes with the drift direction: the step pairs are separated by the terrace A with the step-down drift (a) and by the terrace B with the step-up drift (b).

Figures 1 (c) and (d) represent snap shots of the step bunching in a late stage. Irrespective of the drift direction, the large bunches appear periodically. The wandering fluctuation of the large bunches with the step-down drift is weaker than that with the step-up drift. There are straight step pairs in the large terraces in (c) and no free steps in (d).

The difference of the formation process of bunches is shown in Fig. 2, which represents the time evolution of the average step positions. When the drift is in the step-down direction ( Fig. 2(a)), in the initial stage the step pairs appear and terrace A spreads. The train of step pairs is also unstable and step bunches are produced by the coalescence of step pairs. In a late stage, the coalescence and separation of a receding step pair with advancing large bunches are repeated.

When the drift is in the step-up direction (Fig. 2(b)), the step pairing occurs in the initial stage, which is similar to that with the step-down drift except that the dominant terraces are terrace B. In a late stage large bunches appear as a result of successive coalescence of bunches and there are few free step pairs (one pair in Fig. 2(b)), which repeat coalescence and separation, but the pair moves to the opposite direction compared to (a).

## 4. Summary and discussion

In this paper, by carrying out a Monte Calro simulation, we studied the bunching instability

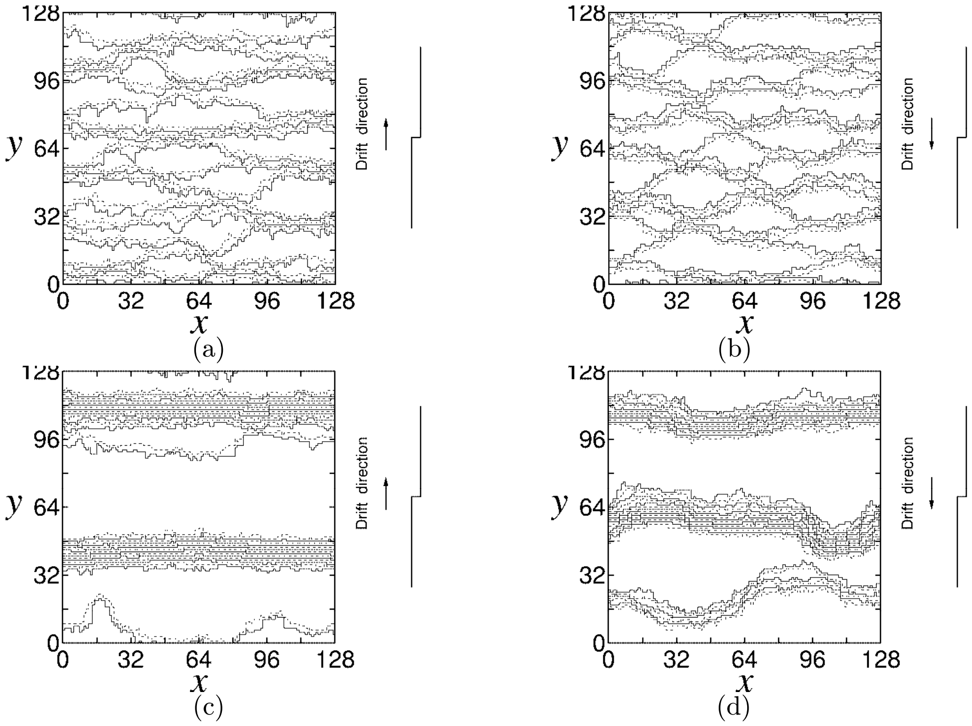


Figure 1. Snap shots of step bunching with anisotropic surface diffusion: (a) with the step-down drift and (b) with the step-up drift in an initial stage, and (c) with the step-down drift and (d) with the step-up drift in a late stage.

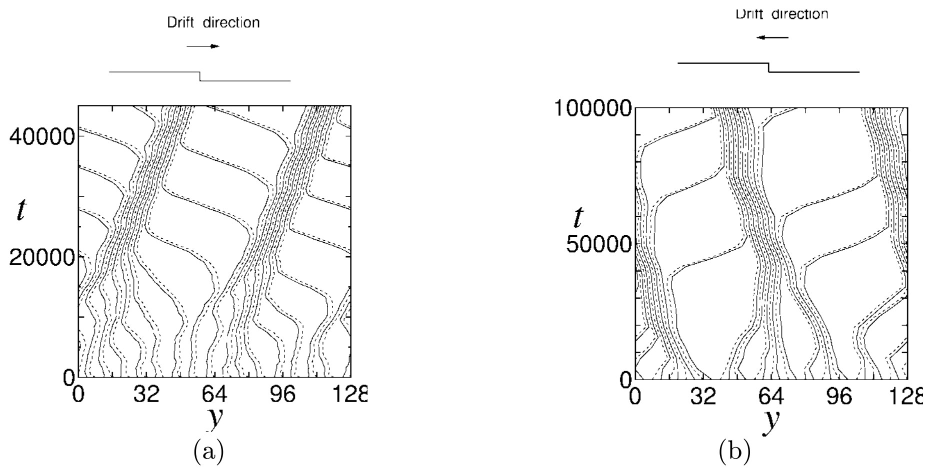


Figure 2. Time evolution of step bunching (a) with the step-down drift and (b) with the step-up drift.

induced by the drift of adatoms with taking account of the anisotropic surface diffusion. In the initial stage of the instability, pairing of steps occurs. The result agrees with the previous stability analysis [4] although the step permeability is different.

In a late stage of the instability, large bunches appear irrespective of the drift direction, while the type of the dominant terraces changes with the drift direction: terrace A with the step-down drift and terrace B with the step-up drift. The result differs from the previous theoretical study [5, 6] where impermeability was assumed. In our simulation we have assumed steps are permeable [7–9], and this difference seems the origin of the discrepancy. Considering the direction of fast diffusion [10, 11] and that the drift is in the current direction [12], our results qualitatively agree with the experiments in Si(001) [1–3], which might imply that the steps are permeable. Since we have also assumed the same step kinetics for the two kinds of steps, we cannot make a definite conclusion for the step permeability in Si(001) yet.


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