Effect of Two-Dimensionality on Step Bunching Induced by the Drift of Adatoms

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We study the effect of two-dimensionality on step bunching induced by drift of adatoms. When anisotropy of the diffusion coefficient changes alternately on consecutive terraces like a Si(001) vicinal face, bunching occurs with the drift of adatoms. If the fluctuation of step bunches is neglected as in the one-dimensional model, the bunching with step-down drift is faster than that with step-up drift in contradiction with the experiment by Latyshev and coworkers. In a two-dimensional model, the step bunches wander heavily with step-up drift and recombination with neighboring bunches occur more frequently than those with step-down drift and the bunching is accelerated. When the difference of kinetic coefficients between two types of steps is taken into account, the bunching with step-up drift can be faster than that with step-down drift.

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I. INTRODUCTION

The Si(001) surface is reconstructed by dimerization of surface atoms. When its vicinal face is tilted in the (110) direction, the terraces with dimer rows parallel to the steps (we call $T_A$) and those with dimer rows perpendicular to the steps (we call $T_B$) appear alternately. Since the surface diffusion along the dimer rows is faster than that perpendicular to the dimer rows, the anisotropy of the surface diffusion changes alternately on consecutive terraces.

On the vicinal face, two types of step instabilities, step wandering and step bunching, occur when a specimen is heated by direct electric current \cite{1,2}. The step wandering occurs with step-up current in the region of relatively large inclination (the tilting angle is $0.08^\circ \leq \theta \leq 0.5^\circ$) \cite{3}. Due to the step wandering, grooves perpendicular to the steps appear on the vicinal face. The step bunching occurs irrespective of the current direction in the region of small inclination ($\theta \leq 0.08^\circ$). The type of dominant terraces, which separate step bunches, is $T_B$ with step-down current and $T_A$ with step-up current. The size of bunch increases with time as $t^{3/2}$ \cite{2}, which is independent of the drift direction. The growth rate of the bunches with step-down current seems slightly slower than that with step-up current.

The step instabilities are caused by drift of adatoms induced by the current. By taking account of alternation of the anisotropic surface diffusion, the step instabilities are theoretically explained. If the repulsive interaction is strong so that the step bunching is suppressed, the step wandering occurs with step-up drift \cite{2}, and straight grooves parallel to the drift appears by in-phase wandering. The motion of the steps is given by the solution of the nonlinear equation derived by Pierre-Louis and co-workers \cite{5}. The step bunching occurs irrespective of the direction of the drift \cite{2,3,4,10,11,12,13,14,15}. Since the current and the drift are in the same direction \cite{12,12}, the results are consistent with the experiments \cite{1,2,3}. In a one-dimensional step flow model \cite{11}, the size of bunches increases with time as $t^{3/2}$ with $\beta$ slightly smaller than 1/2, consistent with the experiment \cite{2}. However, the growth rate with step-up drift is slower than that with step-down drift since terraces with fast diffusion in $y$-direction are dominant with step-down drift. This is in contradiction with the experiment \cite{2}. Since the model with alternating diffusion anisotropy has explained the bunching and the wandering instabilities on the Si(001) vicinal face consistently, this disagreement is a major obstacle to the unified understanding.

In the one-dimensional step flow models \cite{11,10}, the motion of step bunches with step-down drift is similar to that with step-up drift except the time scale. In the Monte Carlo simulation, however, the step pattern is changed by the drift direction \cite{11,11}: the step bunches with step-up drift wander more than that with step-down drift. Such a difference of the step motion in two-dimension may solve the disagreement in the growth rate between the experiment \cite{2} and the one-dimensional model \cite{10}. In this paper, we carry out Monte Carlo simulations and show that the difference of the growth rate vanishes in the two-dimensional model.

II. MODEL

For simplicity, we use a square lattice model with the lattice constant $a = 1$. We take $x$-axis parallel to the steps and $y$-axis in the down-hill 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 positions are single valued functions of $x$.

We repetitively select a solid atom at the step or an...
adatom on the terrace. We perform the diffusion and solidification trial for the adatom and melting trial for the solid atom. In the diffusion trial, the adatom hops to a neighboring site. The anisotropy of the diffusion coefficient and the drift of adatoms are taken into account in the hopping probability. On $T_A$, where the surface diffusion in the $x$-direction is faster, 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 $p_d(1 \pm F_d/k_B T)/4$, where $p_d(<1)$ is the ratio of the two diffusion coefficients. $F_d$ is the force to cause the drift. $F_d > 0$ represents the drift in the down-hill direction. On $T_B$, where the surface diffusion in the $y$-direction is faster, an adatom on the site $(i, j)$ moves to $(i \pm 1, j)$ with the probability $p_d/4$ and to $(i, j \pm 1)$ with the probability $(1 \pm F_d/k_B T)/4$. For a diffusion trial, the time increment is $\Delta t = 1/4N_a$, where $N_a$ is the number of adatoms so that the fast diffusion coefficient is unity.

If the adatom comes in contact with a step from the lower terrace after a diffusion trial, solidification occurs with the probability

$$p_s = \left[1 + \exp\left(\frac{\Delta E_s - \phi}{k_B T}\right)\right]^{-1}.$$  

(1)

$\Delta E_s$ is given by $\Delta E_s = \epsilon \times (the \ increment \ of \ the \ step \ perimeter)$ and $\phi$ is decrement of the chemical potential by solidification. The step stiffness $\beta$ is related to $\epsilon$ as

$$\frac{2\beta}{k_B T} = \sinh^2 \frac{\epsilon}{k_B T}.\quad (2)$$

If we select a solid atom, melting trial is performed. When an adatom is absent on the top of the solid atom, melting occurs with the probability

$$p_m = \left[1 + \exp\left(\frac{\Delta E_m + \phi}{k_B T}\right)\right]^{-1}.$$  

(3)

There is no extra diffusion barrier over the steps: steps are permeable.

III. RESULTS OF SIMULATION

In our simulations, we neglect the long-range repulsive interaction between steps, but take into account a short-range repulsive interaction by forbidding overlap of steps. Impingement of atoms and evaporation are absent.

Figures 1 and 2 represent snapshots of the step bunching. System size is $256 \times 256$ and the number of steps is 64. The parameters are $\epsilon/k_B T = 1.0$, $\phi/k_B T = 1.5$, $F_d/k_B T = \pm 0.08$ and $p_d = 0.5$. Initially a few adatoms are present on the vicinal face. The dotted lines represent $S_A$ steps and the solid lines represent $S_B$ steps.

The vicinal face is unstable with the drift of adatoms. Pairing of $S_A$ and $S_B$ occurs in the initial stage. The upper side step in a pair is $S_A$ with step-up drift and $S_B$ with step-down drift. Small bunches are formed by coalescence of step pairs. Since the stiffness is small, the bunches wander and connect with each other at many places (Fig. 1). From the figures one may have impression that he step with step-down drift are more straight.

The effect of the drift direction on the form of bunches becomes evident in a late stage (Fig. 2). With step-down drift, the bunches are straight and there are few recombination of bunches. With step-up drift, the wandering width of the bunches is large. The bunches collide with each other and frequent recombination is seen. The difference of the form may affect the time evolution of bunch size.

To test the effect of the wandering and recombination on the growth rate, we carry out simulations with a narrow system (Fig. 3). The number of steps is 128 and the system size is $16 \times 512$. We use the parameter $\epsilon/k_B T = 0.5$ for step bunches to wander easily. Other parameters are the same as that in Fig. 2. The wandering of step bunches with step-up drift is suppressed because of the narrow system width. The step bunches are straight irrespective of the drift direction.

In Figure 3, the number $N_{max}$ of steps in the largest bunch at $x = 1$ is plotted as a function of time. The bunches grow by the collisions of straight bunches due to the fluctuation of position of bunches [10, 11]. The growth rate with step-up drift is slower than that with
step-down drift like the one-dimensional model. $N_{\text{max}}$ seems to increase in the power law, $N_{\text{max}} \sim t^\beta$ with $\beta \approx 0.4$ \cite{12}, which is consistent with the one-dimensional result with a combination of $\ln r$ and $r^{-2}$ potentials \cite{11}.

We carry out simulations with a large system size: $512 \times 512$ (Fig. 4). In contrast to the one-dimensional model \cite{11}, the growth of bunch size with step-up drift is as fast as that with step-down drift. Thus the slow diffusion in $y$-direction is compensated by the efficient coalescence by the wandering of bunches.

In the experiment \cite{2}, however, the step bunching with step-up current seems slightly faster than that with step-down current. Additional mechanism to accelerate the bunching with step-up drift may be required. On the Si(001) vicinal face, $S_B$ steps are rougher than $S_A$ steps and the kinetic coefficient is probably larger for $S_B$. We take account of the difference as the probabilities of solidification and melting. At $S_A$, the probability of solidification is assumed to be $r_{ps}$ and that of melting is $r_{pm}$ with $r \leq 1$.

Figure 5 represents the time evolution of bunch size with $r = 0.1$. Other parameters and system size are the same as those in Fig. 4. The growth exponent does not change significantly. The growth rate with step-down drift is suppressed as expected from the reduction factor $r$, but that with step-up drift is slightly enhanced.

In figure 6 we show that the step patterns. As explained already, the bunches with step-down drift are straight. The bunches with step-up drift are wavy and shows more recombination patterns. The reduction of kinetic coefficient of $S_A$ seems to enhance the waviness. As a result, the growth rate with step-up drift becomes faster than that with step-down drift, which is in agreement with the experiment \cite{2}.

IV. SUMMARY AND DISCUSSION

We studied the time evolution of bunch size by Monte Carlo simulation. With step-down drift, the bunches are straight and there are few recombination of bunches. With step-up drift, the bunches wander and recombinations of bunches occur frequently.
In the one-dimensional model\textsuperscript{[10,11]}, the velocity of a bunch is roughly proportional to the diffusion coefficient of $y$-direction in large terraces. Bunches with step-down drift grow faster than those with step-up drift, which is in disagreement with the experiment\textsuperscript{[2]}. In the two-dimensional model, bunches with step-up drift wander and collide with each other more frequently than those with step-down drift. Since coalescence of bunches starts from the connected parts, the step bunching with step-up drift occurs more frequently than that with step-down drift. Also the fast transverse diffusion with step-up drift helps recombination of bunches. Consequently the growth rate of bunches with step-up drift is as fast as that with step-down drift.

When the difference of the kinetic coefficient is taken into account, the bunches with step-up drift grows faster than those with step-down drift. The reversal of the growth rate is thus attributed to the two-dimensional step pattern. Since we have not succeeded in quantifying the effect, it is not clear if the proposed effect is sufficient to explain the experiment\textsuperscript{[2]}.

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\item \textsuperscript{[15]} In the limited size of our simulation, it is difficult to define a bunch size. We regard a step pair as being contained in the bunch if the distance between the step pair and the bunch is smaller than a prescribed value. The obtained exponent, though not very sensitively, depends on the value.
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