Step bunching with alternation of structural parameters

Step Bunching with Alternation of Structural Parameters

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By taking account of the alternation of structural parameters, we study bunching of impermeable steps induced by drift of adatoms on a vicinal face of Si(001). With the alternation of diffusion coefficient, the step bunching occurs irrespective of the direction of the drift if the step distance is large. Like the bunching of permeable steps, the type of large terraces is determined by the drift direction. With step-down drift, step bunches grows faster than those with step-up drift. The ratio of the growth rates is as large as the ratio of the diffusion coefficients. Evaporation of adatoms, which does not cause the step bunching, decreases the difference. If only the alternation of kinetic coefficient is taken into account, the step bunching occurs with step-down drift. In an early stage, the initial fluctuation of the step distance determines the type of large terraces, but in a later stage, the type of large terraces is opposite to the case of alternating diffusion coefficient.

KEYWORDS: step bunching, Si(001) vicinal face, drift of adatoms

1. Introduction

When a Si(001) vicinal face is tilted in the $\langle 110 \rangle$ direction, two types of terraces, 1×2 and 2×1 terraces, appear alternately. In the 1×2 terrace, which we call [1] T_B, the surface diffusion perpendicular to the steps is faster than that parallel to the steps. In the 2×1 terrace, which we call T_A, the relation is opposite.

The two adjacent terraces are separated by a monoatomic height step. The type of the steps also changes alternately: the step at the lower side edge of T_A, which we call S_A, is smoother than that of T_B, which we call S_B. Then, parameters like kinetic coefficient and the step stiffness may change for the two kinds of steps.

When a Si(001) vicinal face is heated by direct electric current, the vicinal face is unstable and step bunching occurs irrespective of the current direction.[2,3] The type of large terraces between bunches is T_B with step-down current and T_A with step-up current. Cause of the step bunching is considered to be the drift of adatoms[4] induced by the current. By using a one-dimensional step model, where the alternation of diffusion coefficient and that of kinetic coefficient are taken into account, Stoyanov[5] theoretically studied the stability of a vicinal face for pairing of steps. With large kinetic coefficients, the step pairing occurs irrespective of the direction of the drift, and the

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type of large terraces between step pairs is determined by the current direction. To study behaviors of step pairs, Natori and co-workers carried out numerical simulation of a similar one-dimensional step model.[6,7] With step-down drift, the step bunching occurs via coalescence of step pairs, but the step bunching does not occur with step-up drift, which disagrees with the experiments.[2,3]

Recently, we carried out Monte Carlo simulation,[8] where the alternation of anisotropic surface diffusion was taken into account. In contrast to the previous studies,[6,7] the step bunching occurs irrespective of the direction of the drift as in the experiment.[2,3] In our model,[8] the steps are perfectly permeable, and the alternation of kinetic coefficient and the evaporation of adatoms are neglected. On the other hand, the steps are impermeable and both the alternation of kinetic coefficient and the evaporation are taken into account in the previous models.[6,7] Since there are many differences between the models, it is not clear what is the most important factor to cause the different results.

In this paper, we use a one-dimensional model of impermeable steps to study the drift-induced step bunching. In Sec. 2, we introduce the model. In Sec. 3, we analyze the model with alternating diffusion coefficient and perform a numerical simulation. We compare the results with our previous study.[8] In Sec. 4, we study the model with the alternating kinetic coefficient. The effect of evaporation, which is neglected in Ref. 8, is also studied in Secs. 3 and 4. In Sec. 5 we summarize the results and give a brief discussion.

2.   Model

We use a one-dimensional step flow model.[5–7] The y-coordinate is taken in the step-down direction. When the drift of adatoms is parallel to the y-axis, the diffusion equation of adatom density $c(y,t)$ is given by

$$\frac{\partial c}{\partial t} = D_m \frac{\partial^2 c}{\partial y^2} - \frac{D_m F}{k_B T} \frac{\partial c}{\partial y} - \frac{1}{\tau} c, \tag{1}$$

where D_m is the diffusion coefficient in the mth terrace, F the force to cause the drift and τ the lifetime of adatoms for evaporation.

Boundary conditions at the mth step are given by[5,9]

$$K_m(c|_+ - c_m) = D_m \left(\frac{\partial c}{\partial y}\bigg|_+ - \frac{F}{k_B T} c|_+ \right)$$
$$- P_m(c|_+ - c|_-), \tag{2}$$

$$K_m(c|_- - c_m) = -D_{m-1} \left(\frac{\partial c}{\partial y}\bigg|_- - \frac{F}{k_B T} c|_- \right)$$
$$- P_m(c|_- - c|_+), \tag{3}$$

where c_m is the equilibrium adatom density, K_m kinetic coefficient of the mth step and $+(-)$ indicates the lower (upper) side of the step. T_A and T_B appear alternately, and we assume steps

with odd numbers are S_B steps and those with even numbers are S_A steps (Figure 1). The diffusion coefficients and the kinetic coefficients are given by $(D_{2n}, K_{2n}) = (D_B, K_A)$ and $(D_{2n-1}, K_{2n-1}) = (D_A, K_B)$. Bearing a Si(001) vicinal face in mind, we set $D_B > D_A$ and $K_B > K_A$. The second terms in the right hand side of eqs. (2) and (3) represent the adatom current through the step without solidification. With $P_m \to \infty$, the difference between $c|_+$ and $c|_-$ vanishes and the step is called perfectly permeable. With $P_m = 0$, the step is called impermeable and the surface diffusion field is separated by the step. Hereafter we deal with the impermeable steps.
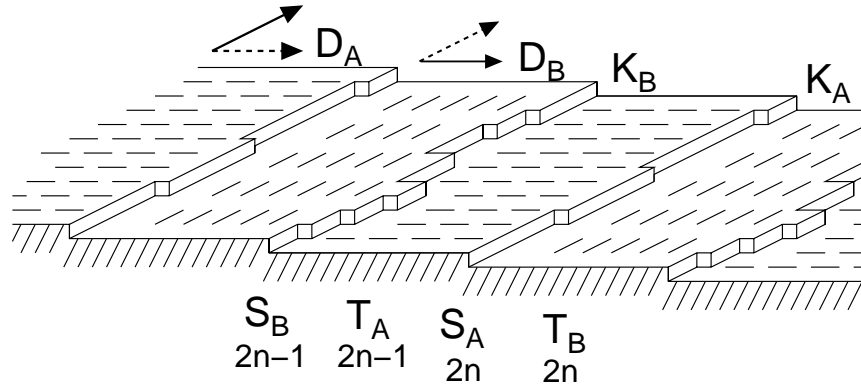

Fig. 1. A restructed Si(001) vicinal face. Short lines represent dimers.

When the neighboring steps interact with the potential ζ_m, the equilibrium adatom density at the mth step c_m is given by[10, 11]

$$
\begin{aligned}
c_m &= c_{\text{eq}}^0 + \frac{\Omega c_{\text{eq}}^0}{k_B T} \frac{\partial \zeta_m}{\partial y_m} \\
&= c_{\text{eq}}^0 \left[1 - \tilde{A}_{\tilde{\nu}} \left(\frac{1}{l_{m-1}^{\tilde{\nu}}} - \frac{1}{l_m^{\tilde{\nu}}} \right) \right]
\end{aligned}
\tag{4}
$$

where c_{eq}^0 is the equilibrium adatom density of an isolated step, Ω the atomic area, y_m the position of the mth step and $l_m = (y_{m+1} - y_m)$ is the width of the mth terrace. If the step interaction potential ζ_m is given by $\zeta_m = -A(\ln l_{m-1} + \ln l_m)$ as in a Si(001) vicinal face,[12] the exponent is $\tilde{\nu} = 1$ and $\tilde{A}_{\tilde{\nu}} = \Omega A / k_B T$.

By solving eq. (1) with the boundary conditions, eqs. (2) and (3), in a quasi-static approximation ($\partial c / \partial t = 0$), we determine the adatom density. The velocity of the mth step is given by

$$
\begin{aligned}
V_m &= K_m(c|_+ - c_m) + K_m(c|_- - c_m) \\
&= \Omega \left(D_m \left. \frac{\partial c}{\partial y} \right|_+ - \frac{D_m F}{k_B T} c|_+ \right) \\
&\quad - \Omega \left(D_{m-1} \left. \frac{\partial c}{\partial y} \right|_- - \frac{D_{m-1} F}{k_B T} c|_- \right).
\end{aligned}
\tag{5}
$$

In the following, to see how the step bunching changes with the alternation of parameters, we separately study the effect of diffusion coefficients and that with kinetic coefficients.

3.   Step bunching with alternation of diffusion coefficient

We use the model of impermeable steps to study the step bunching with alternation of diffusion coefficient. We compare results wtih the previous study[8] to see the effect of step permeability. For simplicity, the alternation of kinetic coefficient is neglected.

3.1   Step bunching induced by drift in a conserved system

We first study the step bunching in a conserved system. Without the evaporation, the step velocity is given by

$$
\begin{aligned}
V_m \quad = \quad & \frac{\Omega K D_{m-1} f(c_{m-1} e^{fl_{m-1}} - c_m)}{(e^{fl_{m-1}} - 1)K + (e^{fl_{m-1}} + 1)D_{m-1}f} \\
& - \frac{\Omega K D_m f(c_m e^{fl_m} - c_{m+1})}{(e^{fl_m} - 1)K + (e^{fl_m} + 1)D_m f},
\end{aligned} \tag{6}
$$

where $f = F/k_B T$.

In a vicinal face with the step distance l, the step velocities are given by

$$
\begin{aligned}
V_{2n} \quad = \quad & -V_{2n-1} \\
= \quad & \frac{\Omega K^2 f c_{eq}^0 (e^{fl} - 1)^2 (D_A - D_B)}{v_A v_B},
\end{aligned} \tag{7}
$$

where v_A and v_B are

$$
\begin{aligned}
v_A \quad &= \quad (e^{fl} - 1)K + (e^{fl} + 1)D_A f, \\
v_B \quad &= \quad (e^{fl} - 1)K + (e^{fl} + 1)D_B f.
\end{aligned} \tag{8}
$$

Since the diffusion coefficient D_B is larger than D_A, S_B steps advance and S_A steps recede with step-down drift ($f > 0$). With step-up drift ($f < 0$), the direction of the step motion is reversed.

In the initial stage of the instability, formation of large $T_B(T_A)$ terrace with step-down (step-up) drift is expected due to the step pairing. To study the motion of pairs of steps, we carry out numerical integration of eq. (6). In addition to the step distance l, there are two characteristic lengths in the vicinal face. One is $f^{-1} \sim k_B T/eE$,[13] which is a characteristic length determined by the drift and usually much larger than the step distance. The other is D_B/K, which is characteristic length determined by step kinetics. When the step distance l is much smaller than D_B/K, the step kinetics is more important than the surface diffusion. We assume that f^{-1} is larger than D_B/K, and study the time evolution in two cases; $D_B/K < l$ and $l < D_B/K$.

Figure 2 represents the time evolution of step positions with $D_B/K \ll l \ll f^{-1}$. This is the case in which the diffusion is slow and controls the time evolution. Solid lines represent the evolution
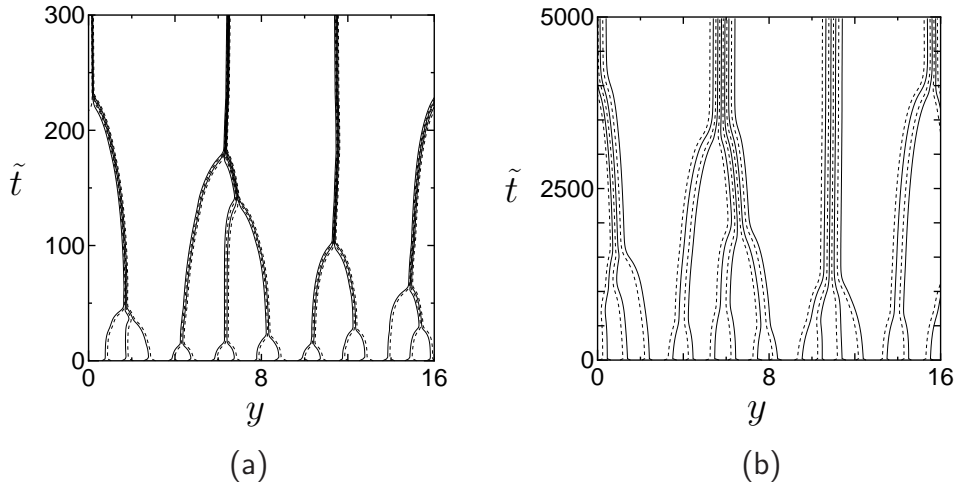
Fig. 2. Time evolution of step position. The step distance l is larger than D_A/K and D_B/K. The drift direction is (a) step-down drift and (b) step-up, and the drift velocities satisfy $|fl| = 0.1$. The number of steps is 32 and the system size is 16 with the periodic boundary condition. $\tilde{A}_{\tilde{\nu}} = 5 \times 10^{-3}$ with $\tilde{\nu} = 1$, $D_B/Kl = 0.2$, $D_A/Kl = 0.02$ and $\tilde{t} \equiv \Omega c_{eq}^0 t$.

of the positions of S_B and dotted lines represent S_A. The characteristic length f^{-1} is $f^{-1} = 200$ and the scaled time $\tilde{t}$ is given by $\tilde{t} \equiv \Omega c_{eq}^0 t$. The initial step distance is about the same, but with a random fluctuation. In the initial stage, the step pairing occurs irrespective of the drift direction. Large terraces are T_B with step-down drift (Fig. 2(a)) and T_A with step-up drift (Fig. 2(b)), which agrees with eq. (7) and the previous analysis.[5–7]

In a later stage, large bunches appear irrespective of the drift direction. The type of large terraces is the same as in the initial stage. Free single steps or pairs do not exist on the large terraces and the bunches grow via coalescence of small bunches. Though the formation process of large bunches is similar in both cases, the step density with step-down drift is higher than that with step-up drift, and the growth is much faster. The ratio of the growth rate of step bunches is as large as the ratio of the diffusion coefficients. In the numerical study of Natori et al.,[6,7] the formation of large bunches with step-up drift did not occur in contrast to our simulation. For the very slow growth rate of step bunches, their simulation time might be too short to produce large bunches.

Figure 3 represents the step bunching with $l \ll D_A/K$, *i.e.*, the step kinetics-control case. The amplitude of the initial fluctuation is the same as that in Fig. 2. When the drift is in the step-down direction (Fig. 3(a)), the equidistant step train is unstable and the step bunching occurs. The terrace type between step bunches is determined by the initial fluctuation and both types of large terraces coexist. When the drift is in the step-up direction (Fig. 3(b)), the step bunching does not seem to occur. The results are very different from Fig. 2.

To find the reason that the step behavior changes with the kinetic coefficients, we analyse the change of alternating terrace width. We assume the width of T_B is $l_{2n} = l + \Delta l/2$ and that of
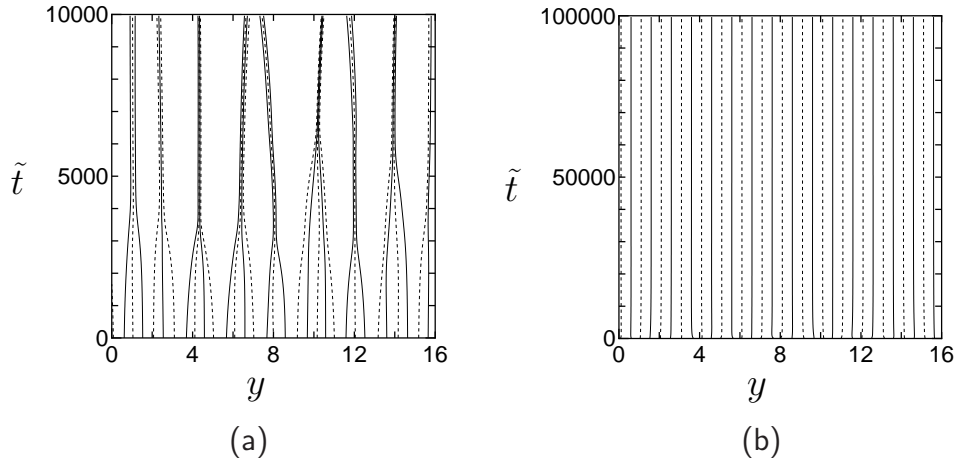
Fig. 3. Time evolution of step position with step distance $l \ll D_A/K, D_B/K$ with (a) step-down drift and (b) step-up drift. The number of steps is 32 and the system size is 16 with the periodic boundary condition. $\tilde{A}_{\tilde{\nu}} = 4 \times 10^{-3}$ with $\tilde{\nu} = 1$, $|fl|$=0.1, $D_B/Kl = 200$ and $D_A/Kl = 20$.
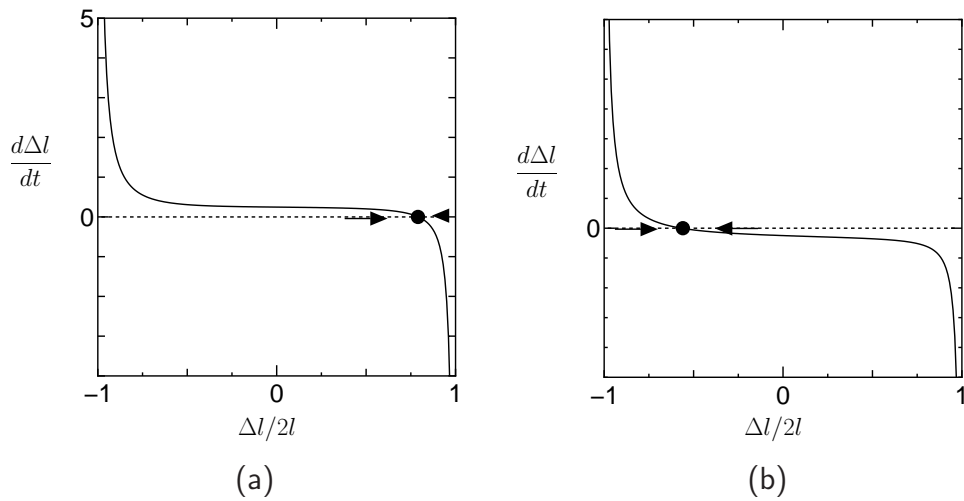

Fig. 4. Time derivative of the terrace width change Δl with (a) step-down drift and (b) step-up drift. Parameters are the same as in Fig. 2.

T_A is $l_{2n-1} = l - \Delta l/2$. Figure 4 represents the time derivative of Δl for large kinetic coefficients. Parameters are the same as in Fig. 2. With step-down drift (Fig. 4(a)), the initial vicinal face $\Delta l = 0$ is unstable and Δl increases up to the stable fixed point near $\Delta l = 2l$. The surface consists of large T_B terraces and small T_A terraces, *i.e.*, tight step pairs. With step-up drift (Fig. 4(b)), the initial stage is also unstable and Δl decreases to the stable fixed point near $\Delta l = -2l$. The surface consists of small T_B terraces and large T_A terraces. The results agree with the initial pairing stage of Fig. 2.

Figure 5 represents the time derivative of Δl for small kinetic coefficients. With step-down drift (Fig. 5(a)), there are three fixed points. The fixed point (open circle) near the center is unstable and two other fixed points (filled circles) are stable. Since the unstable fixed point is very close to $\Delta l = 0$, the final stage is not unique if the initial fluctuation is included. In Fig. 3(a), the initial random fluctuation is not negligible and some terraces move to the fixed point with positive Δl and two types of terraces coexist.
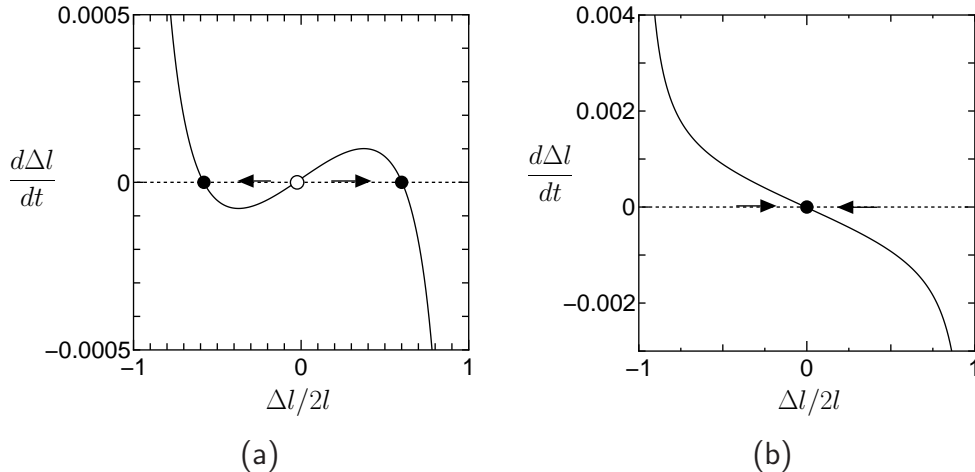

Fig. 5. Time derivative of the terrace width change Δl with (a) step-down drift and (b) step-up drift. Parameters are the same as in Fig. 3.

With step-up drift, there is only one stable fixed point with a small negative Δl. From the condition V_m in eq. (6), the difference of step distance Δl in the fixed point near $\Delta l = 0$ is given by

$$\frac{\Delta l}{l} = \frac{Kl(D_A - D_B)}{2D_A D_B},\tag{9}$$

where we neglected the step-step repulsive interaction. The sign of Δl is determined by the diffusion coefficients and independent of the drift direction as seen in Fig. 3(b).

3.2 Step bunching induced by evaporation

Since the experiments[2,3)] were carried out at high temperatures, the evaporation of adatoms may not be negligible for the step bunching.

We first neglect the drift of adatoms and see if the step bunching occurs with the evaporation. For simplicity, we consider the limit of the fast step kinetics, $K \to \infty$. If the step repulsion is absent, the step velocity is given by

$$\frac{V_m}{\Omega c_{\text{eq}}^0} = -\frac{D_m}{x_m} \tanh \frac{l_m}{2x_m} - \frac{D_{m-1}}{x_{m-1}} \tanh \frac{l_{m-1}}{2x_{m-1}}, \tag{10}$$

where $x_m = \sqrt{D_m \tau}$ is the surface diffusion length in the mth terrace. With the same step distance l, the step velocity is given by

$$
\begin{aligned}
V_{2n} &= V_{2n-1} \\
&= -\Omega c_{\text{eq}}^0 \left[\frac{D_A}{x_A} \tanh \frac{l}{2x_A} + \frac{D_B}{x_B} \tanh \frac{l}{2x_B} \right],
\end{aligned} \tag{11}
$$

where $x_A (x_B)$ represents the surface diffusion length in $T_A (T_B)$ and the equidistant train of steps is a steady state. When the terrace widths change alternately and are given by $l_{2n} = l + \Delta l/2$ and $l_{2n-1} = l - \Delta l/2$, from eq. (10) the time evolution of Δl is given by

$$\frac{1}{2} \frac{d\Delta l}{dt} = V_{2n} - V_{2n-1} = 0. \tag{12}$$

The vicinal face is marginal to the perturbation. If the repulsive interaction is taken into account, the vicinal face is stable and the step pairing does not occur. With the alternation of diffusion coefficient, the evaporation alone does not cause the step bunching.

When both the drift and the evaporation are present, the step velocity is given by

$$
\begin{aligned}
\frac{V_m}{\Omega} =\ & \frac{(D_{m-1} - D_m) f c_m}{2} \\
& - \frac{D_{m-1} \alpha_{m-1} (c_m \cosh \alpha_{m-1} l_{m-1} - e^{-f l_{m-1}/2} c_{m-1})}{\sinh \alpha_{m-1} l_{m-1}} \\
& - \frac{D_m \alpha_m (c_m \cosh \alpha_m l_m - e^{-f l_m/2} c_{m+1})}{\sinh \alpha_m l_m}.
\end{aligned} \tag{13}
$$

The parameter α_m is defined by

$$\alpha_m = \frac{1}{2} \sqrt{f^2 + \frac{4}{x_m^2}}. \tag{14}$$

α_m^{-1} is the characteristic length of the diffusion field in the mth terrace.

We carry out numerical integration of eq. (13). The time evolution of step positions (Figure 6) shows the drift-induced step bunching with the evaporation, where the characteristic length scale in T_B is $\alpha_{2n}^{-1} = 14.9$ and that in T_A is $\alpha_{2n-1}^{-1} = 8.9$. Irrespective of the drift direction, very fast pairing of receding steps occurs at the initial stage. The type of large terraces is the same as in Fig 2 and not changed by the evaporation.

Large bunches appear by coalescence of small bunches. With step-down drift, coalescence of step bunches occurs successively, but the time interval of the coalescence increases with increasing
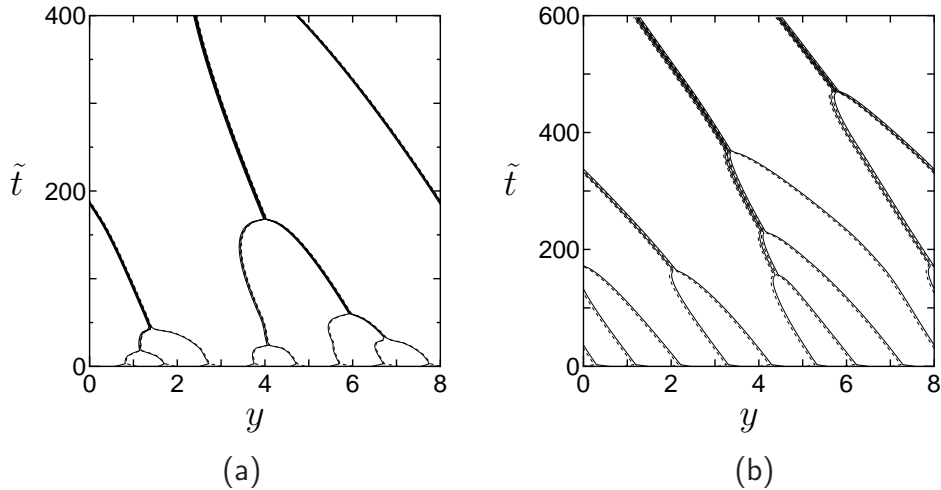
Fig. 6. Time evolution of step position with evaporation with (a) step-down drift and (b) step-up drift. The number of steps is 16 and system size is 8. The diffusion coefficients are $D_A = 2$ and $D_B = 10$. Other parameters are $f = 0.1$ $\nu\Omega A/k_B T = 10^{-4}$ with $\nu = 1$, and $\tau = 50$.

the terrace width between bunches (Fig. 6(a)). With step-up drift, coalescence of step pairs does not occur until $\tilde{t} \approx 150$. However, once the coalescence of step pairs starts, the interval does not seem to increase much (Fig. 6(b)). The difference between the growth rate of bunch size with step-down drift and that with step-up drift is much smaller than that without the evaporation.

4. Step bunching with alternation of kinetic coefficient

In a Si(001) vicinal face, not only diffusion coefficients but also the type of steps changes alternately. In this section, we study the step bunching due to the alternation of kinetic coefficient and compare the result with Sec. 3.

4.1 Step bunching induced by drift

To focus on the alternation of step kinetics, we neglect the alternation of diffusion coefficients. First, we neglect the evaporation. Without the evaporation, the step velocity is given by

$$V_m = \frac{\Omega D_s f K_m K_{m-1}(e^{fl_{m-1}} c_{m-1} - c_m)}{K_{m-1}(D_s f - K_m) + K_m(D_s f + K_{m-1})e^{fl_{m-1}}}$$
$$- \frac{\Omega D_s f K_m K_{m+1}(e^{fl_m} c_m - c_{m+1})}{K_m(D_s f - K_{m+1}) + K_{m+1}(D_s f + K_m)e^{fl_m}}, \tag{15}$$

where D_s is the diffusion coefficient.

In a vicinal face with equidistant steps, the step velocities are given by

$$V_{2n} = -V_{2n-1}$$
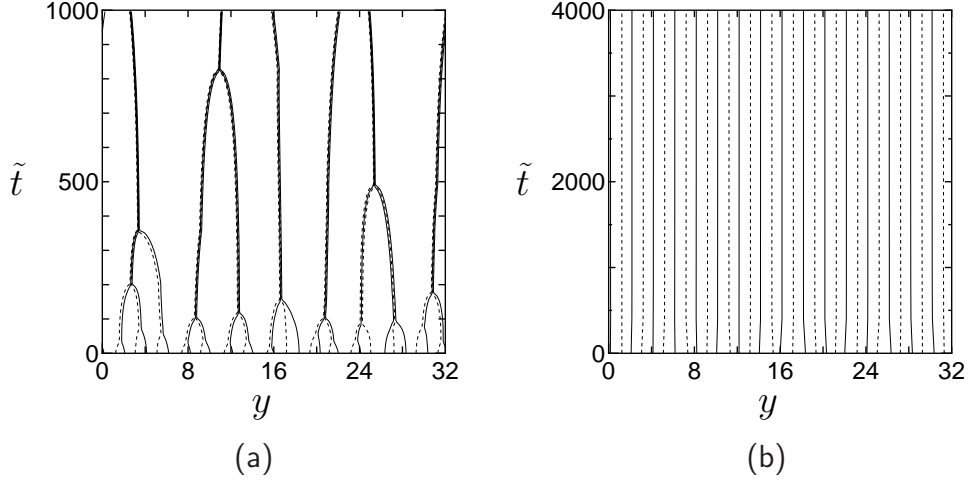$$= \frac{\Omega D_s K_A K_B c_{eq}^0 f^2 (e^{fl} - 1)^2 (K_B - K_A)}{g_A g_B}, \tag{16}$$

Fig. 7. Time evolution of step position with alternating change of kinetic coefficient with step distance $D_s/K_A \ll 1$. Drift is in (a) step-down direction and (b) the step-up direction. The number of steps is 32 and the system size is 32 with the periodic boundary condition. Parameters are $\tilde{A}_{\tilde{\nu}} = 2 \times 10^{-3}$ with $\tilde{\nu} = 1$, $|fl| = 0.2$, $D_s/K_A l = 0.1$. and $D_s/K_B l = 1.0 \times 10^{-2}$.

where g_A and g_B are

$$
\begin{aligned}
g_A &= [K_A(D_s f - K_B) + K_B(D_s f + K_A)e^{fl}], \\
g_B &= [K_B(D_s f - K_A) + K_A(D_s f + K_B)e^{fl}].
\end{aligned}
\tag{17}
$$

Since the kinetic coefficient K_B is larger than K_A, S_A steps advance and S_B steps recede. Alternation of large T_A terraces and small T_B terraces is expected by formation of step pairs.
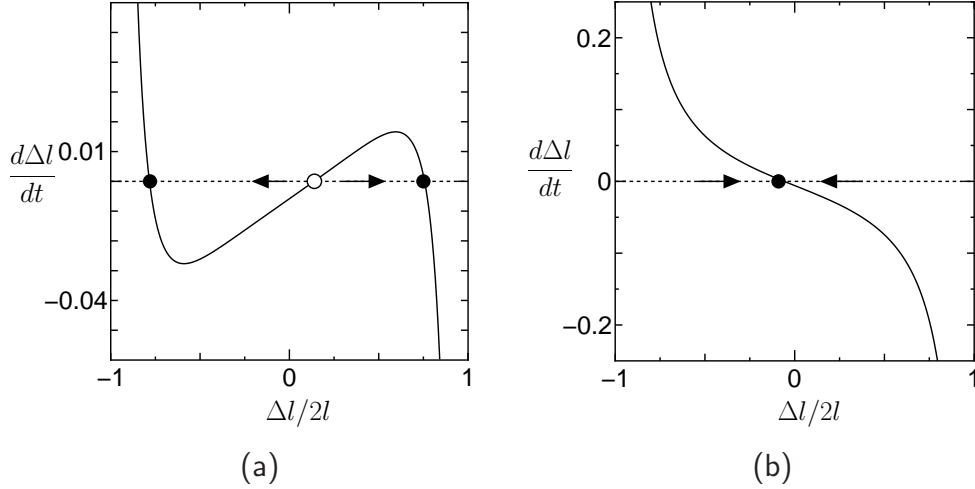

Fig. 8. Time derivative of the terrace width change with (a) step-down drift and (b) step-up drift. Parameters are the same as in Fig. 7

When the kinetic coefficient K_B is large, $D_s/K_B \ll l$, time evolution of step positions is shown in Fig. 7. With step-down drift (Fig. 7(a)), most steps form pairs and large T_A terraces appear in the initial stage, but formation of triplets also occurs and a large T_B is produced. In a later stage,

all large terraces become T_A after coalescence of small bunches. With step-up drift (Fig. 7(b)), the pairing does not seem to occur.

Figure 8 represents the growth rate of Δl, which is defined in the same way as in Sec. 3.1. With step-down drift, an unstable fixed point with a small positive Δl and two stable fixed points with a large amplitude of $|\Delta l|$ are present. From the condition $V_m = 0$ in eq. (15), the difference of terrace width at the fixed point near $\Delta l = 0$ is given by

$$\frac{\Delta l}{l} = \frac{K_A - K_B}{K_A + K_B} fl, \tag{18}$$

where we have used $fl \ll 1$ and neglected the step-step repulsion. In eq. (9) Δl is determined only by structural parameters and independent of the drift, but in eq. (18) Δl depends on the drift and changes the sign with the drift direction. Expect for the sign of Δl in the unstable fixed points, the form of $d\Delta l/dt$ is the same as in Fig. 5. The initial vicinal face moves to the steady state with the large negative Δl if the initial fluctuation is small, but it can move to the other steady state with large Δl if the initial fluctuation is large. In Fig. 7(a), formation of a large T_B in the initial stage is due to a large fluctuation of terrace width.

With step-up drift, there is only one fixed point with a negative Δl. The steady state is stable. Since the difference of terrace width Δl is small, the surface does not look like changing in Fig. 7(b).

With the alternation of diffusion coefficient, the form of $d\Delta l/dt$ changes with decreasing the kinetic coefficients (Figs. 4 and 5). On the other hand, with the alternation of kinetic coefficient, the form of $d\Delta l/dt$ does not change even if D_s/K changes. Thus the bunching behavior is insensitive to the ratio D_s/K.

4.2 Step bunching induced by evaporation

If the evaporation is present and the drift is absent, the step velocity is given by

$$\frac{x_s V_m}{\Omega D_s} = \\ -\frac{(\lambda_{m+1} \sinh l_m/x_s + \cosh l_m/x_s)c_n - c_{n+1}}{h_{m+1}(l_m)} \\ -\frac{(\lambda_{m-1} \sinh l_{m-1}/x_s + \cosh l_{m-1}/x_s)c_n - c_{n-1}}{h_m(l_{m-1})}, \tag{19}$$

where $\lambda_m = D_s/K_m x_s$, and $h_m(l)$ is

$$\begin{aligned} h_m(l) &= (\lambda_{m-1}\lambda_m + 1)\sinh l/x_s \\ &+ (\lambda_m + \lambda_{m-1})\cosh l/x_s. \end{aligned} \tag{20}$$

Due to the evaporation, both S_A steps and S_B steps recede. When the steps are equidistant, the difference of step velocities is given by

$$V_{2n} - V_{2n-1} = \frac{(\lambda_A - \lambda_B)\tanh l/x_s}{(1 + \lambda_A\lambda_B)\tanh l/x_s + (\lambda_A + \lambda_B)}. \tag{21}$$

Since λ_A is smaller than λ_B, S_B recedes faster than S_A. The vicinal face is unstable, and large T_A terraces and small T_B terraces appear by step pairing.
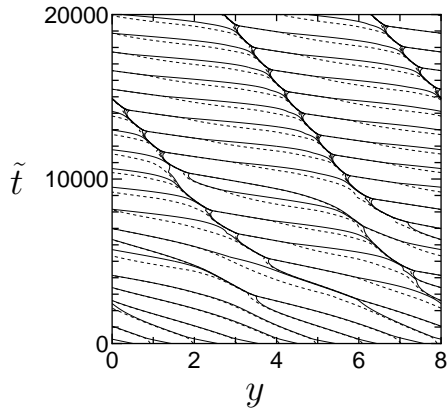

Fig. 9. Time evolution of step position. $x_s = 15$, $K_A = 0.125$, $K_B = 1.0$, $D_s = 1.0$. The number of step is 16 and the system size is 8 with the periodic boundary condition. $\tilde{A}_{\tilde{\nu}} = \times 10^{-4}$ with $\tilde{\nu} = 1$.

Figure 9 represents the time evolution of step positions, which is obtained by numerical integration of eq. (19). In the simulation, the difference of kinetic coefficients is very large. In very early stage, pairing of steps occurs and large T_A terraces appear. Via coalescence of step pairs, step bunches appear. The type of large terrace is the same as that in the step bunching induced by the drift. In large terraces, isolated step pairs are present. When a collision between a step bunch and a step pair occurs, another step pair leaves from the upper side of the step bunch. A step pair breaks into single steps, but only temporarily. Repeating of such collisions is seen in other bucnhing systems.[15, 16] Here a step pair is the fundamental unit.

5.   Summary and Discussion

In this paper, we studied the drift-induced step bunching with the alternation of structural parameters: the diffusion coefficient and the kinetic coefficient.

With the alternation of diffusion coefficients on consecutive terraces, the step bunching occurs irrespective of the drift direction if the kinetic coefficients are large. The type of large terraces is determined by the drift direction. When the kinetic coefficients are small, the step bunching occurs with step-down drift and the initial fluctuation of step distance influences the type of step pairs. The growth rate of bunch size with the step-down drift is much faster than that with the step-up drift, but the difference of growth rates decreases with the evaporation. Without drift of adatoms, the evaporation does not induce bunching.

With the alternation of kinetic coefficient at consecutive steps, the step bunching occurs with the step-down drift and does not occur with the step-up drift. The type of large terraces is influenced by the initial fluctuation of step distance. The evaporation induces step bunching even if the drift

is absent, in contrast to the case with the alternation of the diffusion coefficient.

In the experiments,[2,3] the type of terraces between bunches changes with the drift direction when the initial step distance is large. From our result we may conclude that the alternation of the diffusion coefficient is essential to the bunching and that of kinetic coefficient is not so important. Also the kinetic coefficients are large if the steps are impermeable. Impermeable steps with large kinetic coefficients are effectively equivalent to the permeable steps.[8,18] However, when the step distance is smaller than the critical value, the step bunching occurs only with the step-up current in the experiment,[2] which is not explained by our model. In the previous studies,[18,19] the dift direction to cause the step bunching on a Si(111) vicinal face is affected by the step permeability. In a similar way, the disagreement in a Si(001) vicinal face may be explained by the step permeability, which remains to be explored.

The difference of growth rate of step bunches as the change of current direction is very small in the experiment[3] in contrast to the present result. The evaporation probably plays an important role, but the difference does not vanish only with the evaporation. In the Monte Carlo simulation,[8] in which steps are permeable and evaporation is neglected, the bunches also grow faster with step-down drift. In addition, the two-dimensional step pattern changes with the drift direction. The bunches are straight with step-down drift and wandering with step-up drift. The difference of the two-dimensional motion may reduce the difference of the growth rate for a large system (the system size of the Monte Carlo simulation is very limited). In any case, all these effects are not strong enough to eliminate such a large difference, and we still do not understand the origin of the disagreement.

Acknowledgments

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