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Growth of Step Bunches on a Si(001) Vicinal Face with Drift of Adatoms

Masahide Sato,[*] Tomonori Mori[a], Makio Uwaha[b], and Yukio Hirose[a]

Information Media Center of Kanazawa University,

Kakuma-machi, Kanazawa 920-1192, Japan

[a]*Department of Computational Science, Kanazawa University,*

Kakuma-machi, Kanazawa 920-1192, Japan

[b]*Department of Physics, Nagoya University,*

Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan

Abstract

On a Si(001) vicinal face, where the direction of fast surface diffusion alternates on consecutive terraces, step bunching has been observed under direct current heating. By using a one-dimensional step model with drift of adatoms, we study growth laws of step bunches. If evaporation is negligible, the average number N of steps in a bunch increases with time as $N \propto t^\beta$ with $\beta \lessgtr 1/2$. The growth exponent β weakly depends on the repulsive interaction potential between steps. When steps at a distance l interact with the repulsive potential $\zeta \propto 1/l^\nu$, the average step distance in a bunch l_b decreases as $l_\mathrm{b} \propto N^{-\alpha}$ with $\alpha \approx 3/2(\nu + 2)$. The exponents α and β are related as $\beta \approx 1/(2 + \alpha)$. The simulation results are consistent with experiment if we take account of both logarithmic and $\nu = 2$ potentials, which are expected in this system. The growth rate of the bunch size with step-down drift is faster than that with step-up drift. If evaporation of adatoms is significant, the difference of the growth rate in the opposite drift directions becomes small. The apparent exponent β depends on the drift direction, and is larger with step-up drift.

PACS numbers: step bunching, Si(001) vicinal face, drift of adatoms, growth law

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[*]Electronic address: `sato@cs.s.kanazawa-u.ac.jp`

I. INTRODUCTION

On a Si(001) vicinal face, the surface is reconstructed by dimerization of surface atoms. Due to the dimerization, the surface diffusion is anisotropic and adsorbed atoms (adatoms) move faster along dimer rows than perpendicular to those. When the vicinal face is tilted in the $\langle 110 \rangle$ direction, dimer rows are parallel or perpendicular to the steps and terraces with 1×2 structure and those with 2×1 structure appear alternately. The diffusion coefficient perpendicular to the steps changes alternately.

When a Si(001) vicinal face is heated by direct electric current [1, 2], the vicinal face is unstable and step bunching occurs irrespective of the current direction. The type of large terrace between bunches changes with the current direction. The cause of the step bunching is considered to be drift of adatoms induced by the current [3]. By taking account of the drift in a one-dimensional step model, Stoyanov [4] theoretically studied the stability of the vicinal face, and showed that pairing of steps occurs if the diffusion coefficient perpendicular to the steps changes alternately. The behavior of step pairs has been studied numerically [5–8]. In our previous studies [7, 8], we showed that large step bunches grow and the type of large terrace between bunches is determined by the drift direction, which agrees with the experiments [1, 2].

In the experiment [2], Latyshev and co-workers found growth laws of steps on a Si(001) vicinal face. The number of steps N in a bunch increases with time as $N \propto t^\beta$ with $\beta \approx 1/2$, and the average step distance l_{b} in a bunch decreases as $l_{\mathrm{b}} \propto N^{-\alpha}$ with $\alpha \approx 1/2$.

On a Si(111) vicinal face, the growth laws have been studied theoretically [9–12] and the results agree with the experiments [13–16]. However, the growth laws on a Si(001) vicinal face have not been studied. In this paper, with the Si(001) vicinal face in mind, we study the growth laws in the drift-induced step bunching with the alternating diffusion coefficient. In Sec. II, we introduce a one-dimensional step flow model. In Sec. III we carry out numerical simulation, and find the growth laws of the bunch size and the average step distance. In Sec. IV we summarize results with a brief discussion.

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II. MODEL

We use a one-dimensional step flow model in which the drift of adatoms is taken into account. We consider a vicinal face, where the y-axis is in the step-down direction. On the mth terrace, adatoms diffuse with the diffusion coefficient D_m and evaporate with the lifetime τ. Impingement of atoms is neglected. We assume that the drift is in the y-direction. The diffusion equation of the adatom density $c(y, t)$ is given by

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

where F is the force to cause the drift.

Solidification and melting of atoms occur at steps. In our previous studies [7, 8], we found that the step bunching occurs as observed in the experiment [2] if the kinetic coefficient of steps is large. In this paper we consider the limit of large kinetic coefficient, where the permeable step and the impermeable step are indistinguishable. The adatom density is in equilibrium with steps at the step position:

$$c\big|_{y_m \pm} = c_m, \tag{2}$$

where y_m is the position of the mth step, $+(-)$ indicates the lower(upper) side terrace and c_m is the equilibrium adatom density of the mth step.

On a Si(001) vicinal face, the two kinds of terraces are separated by monoatomic height steps. The alternation of structural anisotropy of terraces produces elastic force monopoles at the steps. The repulsive potential ζ_m is given by $\zeta_m = -A_0 \ln l_m$ [17], where $l_m = (y_{m+1} - y_m)$ is the terrace width.

When the repulsive interaction is taken into account, the equilibrium adatom density is given by

$$\begin{aligned}
c_m &= c_{\mathrm{eq}}^0 \left(1 + \frac{\Omega}{k_{\mathrm{B}} T} \sum_n \frac{\partial \zeta_n}{\partial y_m} \right) \\
&= c_{\mathrm{eq}}^0 \left[1 + \tilde{A}_\nu \left(\frac{1}{l_{m-1}^{\nu+1}} - \frac{1}{l_m^{\nu+1}} \right) \right],
\end{aligned} \tag{3}$$

where c_{eq}^0 is the equilibrium adatom density of an isolated step, and Ω the atomic area. The parameters $\tilde{A}$ and ν in eq. (3) are given by $\tilde{A}_\nu = \Omega A_0 / k_{\mathrm{B}} T$ and $\nu = 0$. In order to study the dependence of the growth laws on the step interaction, we also carry out numerical

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simulation with various potentials, $\zeta_m = A_\nu l_m^{-\nu}$. The parameters $\tilde{A}_\nu$ and A_ν are related by $\tilde{A}_\nu = \nu \Omega A_\nu / k_{\mathrm{B}} T$.

We solve the diffusion equation, eq. (1), with the boundary conditions, eqs. (2) and (3). By using the quasi-static approximation ($\partial c / \partial t = 0$), we obtain the adatom density $c(y)$. The adatom current j_m on the mth terrace is given by

$$j_m = -D_m \frac{\partial c}{\partial y} + \frac{D_m F}{k_{\mathrm{B}} T} c, \tag{4}$$

and the velocity of mth step V_m is

$$\begin{aligned} V_m &= \Omega \left(-j_m\big|_{y_m+} + j_{m-1}\big|_{y_m-} \right) \\ &= \Omega \left(D_m \frac{\partial c}{\partial y}\bigg|_{y_m+} - D_{m-1} \frac{\partial c}{\partial y}\bigg|_{y_m-} \right), \end{aligned} \tag{5}$$

where the terms proportional to the drift vanish because $c\big|_{y_m+} = c\big|_{y_m-} = c_m$. Calculating the step velocity eq. (5) numerically, we can trace the positions of steps.
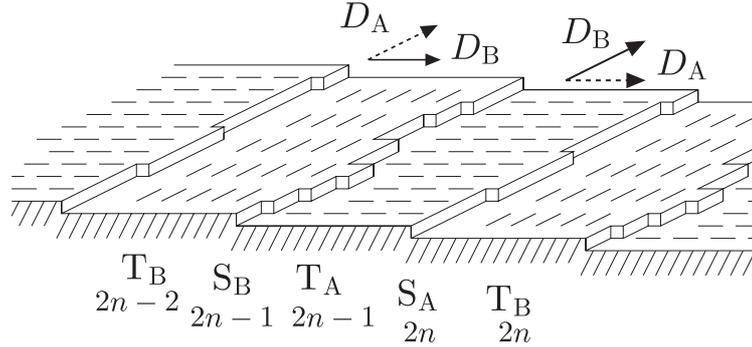
FIG. 1: A Si(001) vicinal face. Short lines represent dimers.

In the following we assume that two types of terraces with different diffusion coefficient appear alternately as in Si(001) (Fig. 1). On the odd number terraces dimer rows are in the x-direction, and on the even number terraces dimer rows are in the y-direction. We call the odd number terraces T_{A} and the even number terraces T_{B}. In the y-direction, the diffusion coefficient D_{A} in T_{A} is smaller than that D_{B} in T_{B}. The lower side step of T_{A} is called S_{A} and that of T_{B} is called S_{B}.

III. SIMULATION RESULTS

In this section we summarize the result of numerical simulations. We first neglect the evaporation and find the growth laws in a conserved system, where the results are simple. Then we study how evaporation influences the growth laws.

A. Step bunching without evaporation

Without evaporation ($\tau \to \infty$), the step velocity is given by [11]

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

where $f = F/k_{\mathrm{B}}T$. f^{-1} represents the characteristic length of the drift force.

For an equidistant step train, the step velocity is given by

$$
V_{\mathrm{A}} = -V_{\mathrm{B}} = (D_{\mathrm{A}} - D_{\mathrm{B}})f.
\tag{7}
$$

$\mathrm{S_A}$ recedes and $\mathrm{S_B}$ advances with step-down drift ($f > 0$). The step motion is reversed with step-up drift ($f < 0$). Neighboring steps move in the opposite direction and the pairing of steps occurs [4–8]. The repulsive step-step interaction, which forbids the formation of double atomic height steps, causes the change of the equilibrium adatom density. In a step pair, the equilibrium adatom density of the upper side step is larger than that of the lower side step.

Figure 2 shows the time evolution of step positions. The dotted lines represent the motion of $\mathrm{S_A}$ and the solid lines represent that of $\mathrm{S_B}$. The scaled time is defined as $\tilde{t} = \Omega c_{\mathrm{eq}}^0 t$. The characteristic length is $f^{-1} = 5$ and the initial step distance is $l = 0.5$ with a small random fluctuation. In the initial stage, step pairing occurs as expected by the stability analysis. Small bunches are produced via coalescence of step pairs.

The coalescence is induced by the fluctuation of terrace width between step pairs. When the drift is weak enough, $fL \ll 1$, the adatom current $j(L)$ on a large terrace is approximately given by [11]

$$
j(L) \approx -D_L \frac{\Delta c}{L} + D_L f c_{\mathrm{eq}}^0,
\tag{8}
$$
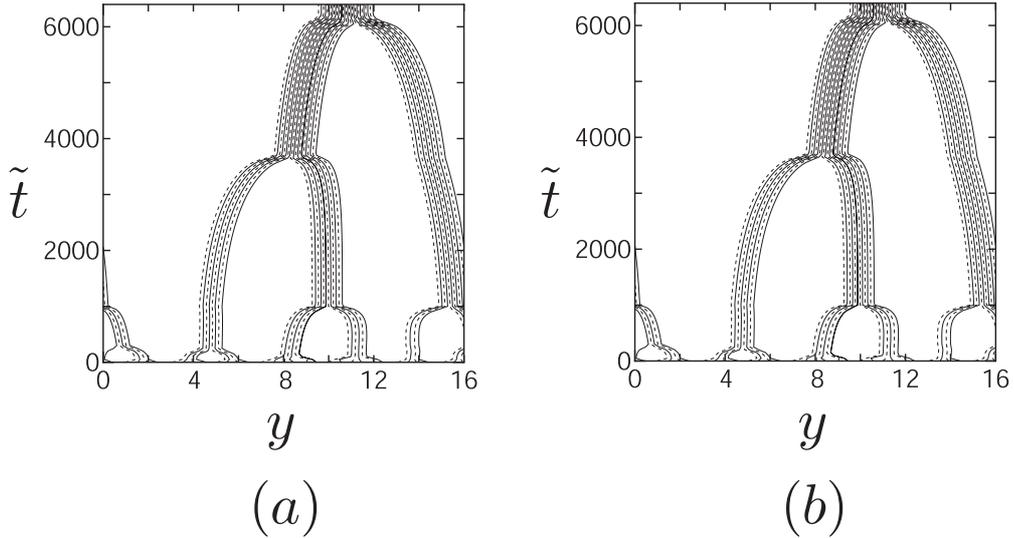
FIG. 2: Time evolution of the step positions in a conserved system with (a) step-down drift and (b) step-up drift. The number of steps is 32. Parameters are $D_B = 2$, $D_A = 1$, $\tilde{A}_2 = 10^{-4}$ with $\nu = 2$, and $f = 0.2$.

where D_L is the diffusion coefficient on the large terrace and Δc is the difference of the equilibrium adatom density in a step pair. The current direction of the second term depends on the drift direction, but that of the first term is always in the step-up direction. When the terrace width between step pairs is much larger than the step distance in a pair, the change of Δc is determined by the step distance in the pair. If the terrace of the width $L + \delta L$ and that of $L - \delta L$ appear alternately, the velocity of step pair whose upper side terrace is larger is given by

$$
\begin{aligned}
V_{\text{pair}} &= \Omega[j(L + \delta L) - j(L - \delta L)] \\
&\approx 2\Omega \frac{\mathrm{d}j(L)}{\mathrm{d}L}\delta L = 2\Omega D_L \frac{\Delta c}{L^2}\delta L.
\end{aligned} \tag{9}
$$

The step pair advances and the fluctuation of terrace width increases. The other step pair with a small upper terrace recedes and the bunching of the step pairs occurs. This process is repeated for larger step bunches successively. In a later stage, very large bunches are produced successively via coalescence of small ones. The process of the step bunching is similar to that on a Si(111) vicinal face [11, 12] except that the step bunching occurs irrespective of the drift direction. The large terrace between bunches is T_B with step-down drift (Fig. 2(a)) and T_A with step-up drift (Fig. 2(b)). The step bunches with step-down drift grow faster than those with step-up drift. When the number of steps is the same, the

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width of the bunch with step-up drift is larger than that with step-down drift.
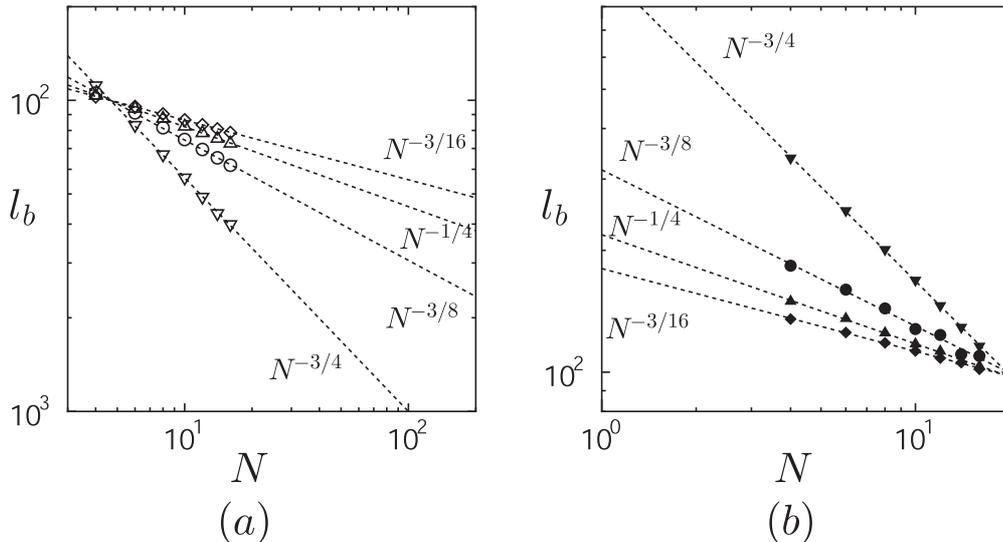
FIG. 3: Dependence of l_b on N. (a) With step-down drift, $\triangledown$ $\nu = 0$ and $\tilde{A}_0 = 10^{-3}$, $\bigcirc$ $\nu = 2$ and $\tilde{A}_2 = 10^{-7}$, $\triangle$ with $\nu = 4$ and $\tilde{A}_4 = 10^{-11}$, and $\diamondsuit$ with $\nu = 6$ and $\tilde{A}_6 = 10^{-15}$. (b) With step-up drift. Other parameters are $|f| = 1.0$, $D_A = 1$, $D_B = 0.1$.

Figure 3 represents the dependence of l_b on the bunch size N. In order to get better statistics, we performed simulations of a different initial condition [18]. We produced a tight isolated bunch of the size N with various potentials and measured l_b. With increasing the bunch size, the average step distance l_b decreases as $l_b \sim N^{-\alpha}$. The exponent α decreases with increasing the exponent ν of the repulsion, and seems to fit the simple formula

$$\alpha \approx \frac{3}{2(\nu + 2)}. \tag{10}$$

If the drift velocity is the same, the bunch with step-down drift is tighter than that with step-up drift, but the exponent α is the same.

In an isolated bunch, the step distance is small and the adatom current is approximately given by

$$j_m = D_m \frac{c_{m+1} - c_m}{l_m} + D_m f c_m \tag{11}$$

where we have numbered the steps from the left to the right, $m = 1$ to N. One may neglect the change of equilibrium density in the second drift term if the bunch is not too large so that the density change is relatively small. In the steady state of a conserved system, the

adatom current is a constant j_0 on all terraces,

$$j_m = j_0. \tag{12}$$

If the bunch is isolated in an infinite system, far from the bunch the adatom density is c_{eq}^0 and the gradient of the adatom density vanishes. The adatom current j_0 is given by

$$j_0 = D_L f c_{\text{eq}}^0. \tag{13}$$

When the bunches appear periodically, the gradient of the adatom density does not vanish on a large terrace. The adatom current j_0 is slightly smaller than $D_L f c_{\text{eq}}^0$.

Since the diffusion coefficient D_m alternates on consecutive terraces, the first diffusion term in eq. (11) should compensate the change of the drift current to keep the current constant. Thus on terraces between $2n$th and $(2n+1)$th steps, where $D_{2n} = D_L$, the second term in eq. (11) is as large as j_0 and the gradient term is very small. On terraces between $(2n-1)$th and $2n$th steps, where $D_{2n-1} \neq D_L$, the difference between the second term and j_0 is large. Thus the diffusion current, which is in the step-down direction, does not vanish. The density change $c_{2n-1} - c_{2n}$ is positive and large.
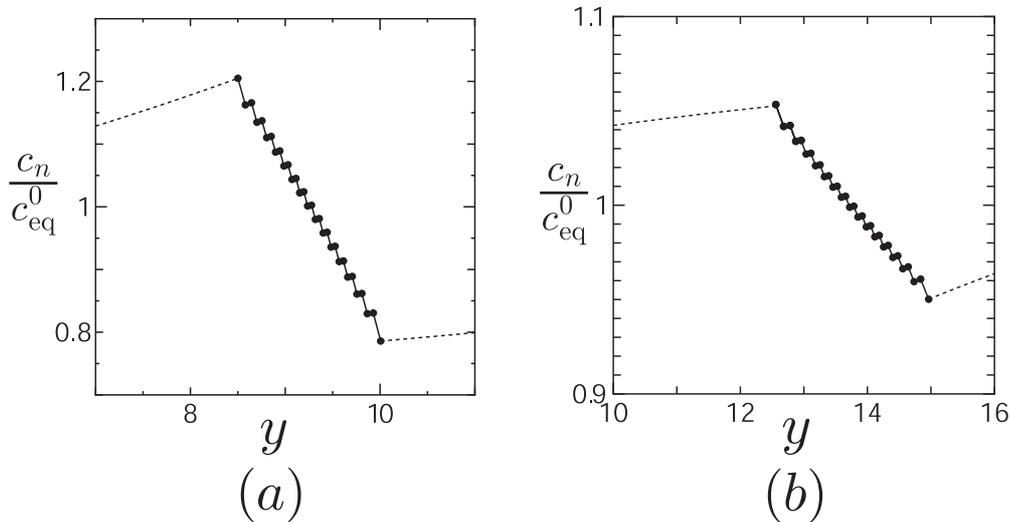
FIG. 4: The equilibrium adatom density in a bunch with (a) step-down drift and (b) step-up drift. Parameters are $D_{\text{A}} = 1.0$, $D_{\text{B}} = 0.1$, $\tilde{A}_2 = 10^{-4}$ with $\nu = 2$, and $|f| = 0.1$.

We were not able to solve eq. (11) with alternating D_m analytically. In Figure 4 we show the density profile in a bunch calculated numerically. The difference of the equilibrium adatom density is large on the odd number terraces, which are terraces in the original step

pairs, in contrast to the even number terraces. From the observation that the diffusion current on the odd number terraces are approximately constant $(c_{2n-1} - c_{2n})/l_{2n-1} \approx$ const., we conjecture that the following relation holds:

$$\Delta c_B \equiv c_1 - c_N \sim \sum_{n=1}^{N/2} (c_{2n-1} - c_{2n}) \propto l_b N \propto N^{1-\alpha}. \tag{14}$$
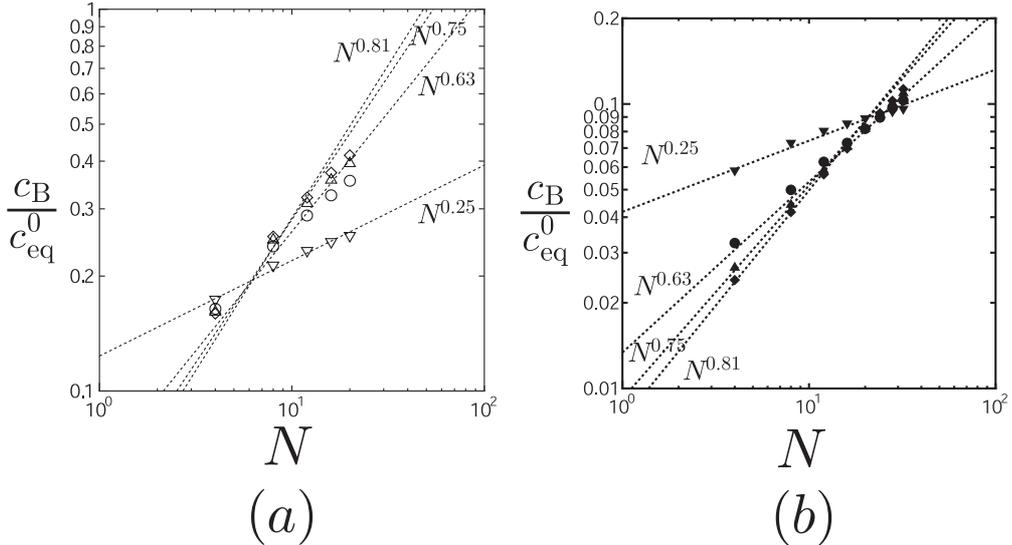
FIG. 5: Dependence of Δc_B on N in Fig. 3 with (a) step-down drift and (b) step-up drift.

Figure 5 shows the difference Δc_B of the equilibrium adatom density between the upper side edge and the lower side edge. It increases in a power of N. When the drift is in the step-down direction (Fig. 5(a)), the exponent is smaller than that given by eqs. (10) and (14). This is probably because the change of the equilibrium adatom density is too large ($\Delta c_B/c_{eq}^0 \approx 0.4$). When the drift is in the step-up direction (Fig. 5(b)), change of the equilibrium adatom density is small ($\Delta c_B/c_{eq}^0 \approx 0.1$) and the exponent roughly agrees with the expected value: $(2\nu + 1)/(2\nu + 4) = 0.25, 0.625, 0.75, 0.8125$ for $\nu = 0, 2, 4, 6$, respectively.

Since the bunching proceeds hierarchically as observed in Fig. 3, we can estimate the time τ_b necessary for the bunch to double [12]. For a periodic array of N step bunches, pairing instability occurs if the bunch position is shifted alternately. In a similar way to eq. (9), the velocity of the bunch is given by

$$V_{bunch} \sim \Omega D_L \frac{\Delta c_B}{N L^2} \delta L. \tag{15}$$

Then the time necessary for a pair of bunches to collide is

$$\tau_{\mathrm{b}} \sim \frac{NL^2}{\Omega D_L \Delta c_{\mathrm{B}}} \sim N^{2+\alpha}. \tag{16}$$

This hierarchical collision of bunches leads to the growth law of the bunch size as

$$N \sim t^{\beta} \tag{17}$$

with the exponent

$$\beta = \frac{1}{2+\alpha}. \tag{18}$$
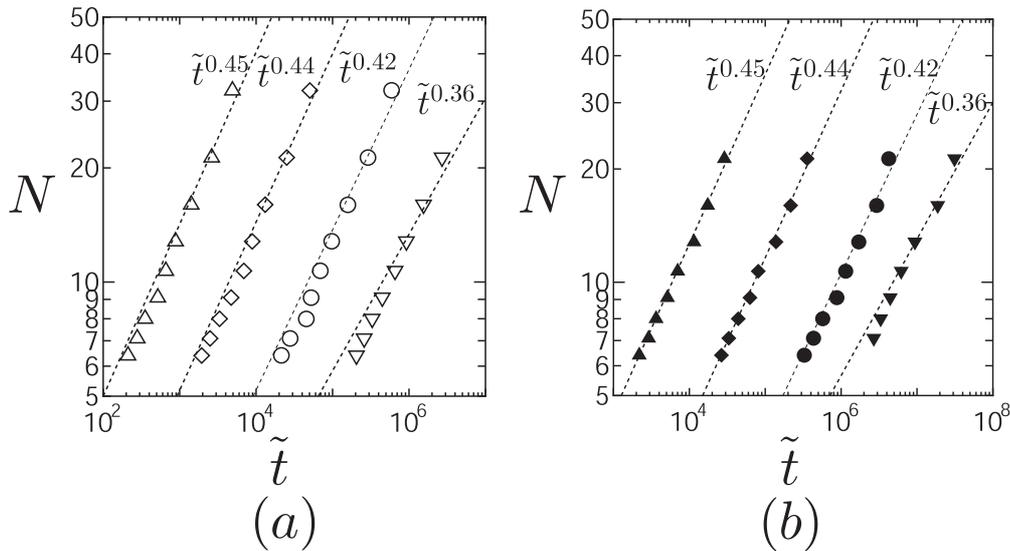
FIG. 6: Time dependence of the bunch size with various repulsive potential with (a) step-down drift and (b) step-up drift. The exponent of the repulsive potential is $\triangledown \nu = 0$, $\bigcirc \nu = 2$, $\triangle \nu = 4$ and $\diamondsuit \nu = 6$.

The growth law eqs. (17) and (18) is tested by the numerical simulation. Figure 6 shows the time dependence of the bunch size N. The simulation is carried out with 64 steps with the initial step distance 0.5. The force to cause the drift is $|f| = 0.1$, and the diffusion coefficients are $D_{\mathrm{A}} = 1.0$ and $D_{\mathrm{B}} = 0.1$. The strength $\tilde{A}$ of the repulsive potential is adjusted to make the bunches to be tight; $\tilde{A}_0 = 10^{-2}$ for $\nu = 0$, $\tilde{A}_2 = 10^{-4}$ for $\nu = 2$, $\tilde{A}_4 = 10^{-5}$ for $\nu = 4$ and $\tilde{A}_6 = 10^{-6}$ for $\nu = 6$. The step number N is averaged in each sample and over 20 runs. The time axis of the data are shifted by $10^{(6-\nu)/2}$ times for each power of the potential ν. The dotted lines indicate the power

$$\beta = \frac{2(\nu+2)}{4\nu+11} \tag{19}$$

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obtained from eq. (18) with the empirical values of eq. (10). For $\nu = 0$ the slope looks slightly larger than the expected value $\beta = 0.36$. Since the ν dependence of the exponent β is weak, it is difficult to use the experimental data to determine the power of the potential. In the experiment [2] β seems to be 0.5, but we do not think the exponent about 0.4 is excluded by the experiment.

B. Step bunching with evaporation

In our previous study [8] for the simple one-dimensional step model, the difference of the growth rate with the change of the drift direction is suppressed considerably by evaporation of adatoms. Here we study the effect of evaporation (finite τ) on the growth laws.

If evaporation is taken into account, the step velocity is given by

$$
\begin{aligned}
\frac{V_m}{\Omega} &= \frac{(D_{m-1} - D_m)fc_m}{2} \\
&- \frac{D_{m-1}\alpha_{m-1}(c_m \cosh \alpha_{m-1}l_{m-1} - e^{-fl_{m-1}/2}c_{m-1})}{\sinh \alpha_{m-1}l_{m-1}} \\
&- \frac{D_m\alpha_m(c_m \cosh \alpha_m l_m - e^{-fl_m/2}c_{m+1})}{\sinh \alpha_m l_m}.
\end{aligned}
\tag{20}
$$

The parameter α_m is defined as

$$
\alpha_m = \frac{1}{2}\sqrt{f^2 + \frac{4}{x_m^2}},
\tag{21}
$$

where $x_m = \sqrt{D_m \tau}$ is the surface diffusion length in the mth terrace. The parameter α_m^{-1} is the characteristic length of the surface diffusion in the mth terrace. It decreases as the evaporation increases. If the step distance is larger than α_m^{-1}, the interaction between steps mediated by the surface diffusion is weak.

Figure 7 represents time evolution of step positions with evaporation. The lifetime is $\tau = 80$ and the characteristic lengths are $\alpha_B^{-1} = 7.8$ and $\alpha_A^{-1} = 6.7$. Step bunches grow via successive coalescence of small bunches similarly to the conserved system. In the initial stage, coalescence of step bunches with step-down drift (Fig. 7(a)) occurs faster than that with step-up drift (Fig. 7(b)). In a later stage, however, the coalescence with step-up drift is more frequent than that with step-down drift. The size of step bunches with step-up drift catches up with that with step-down drift. In both cases a large isolated bunch is formed at $\tilde{t} \approx 3000$.
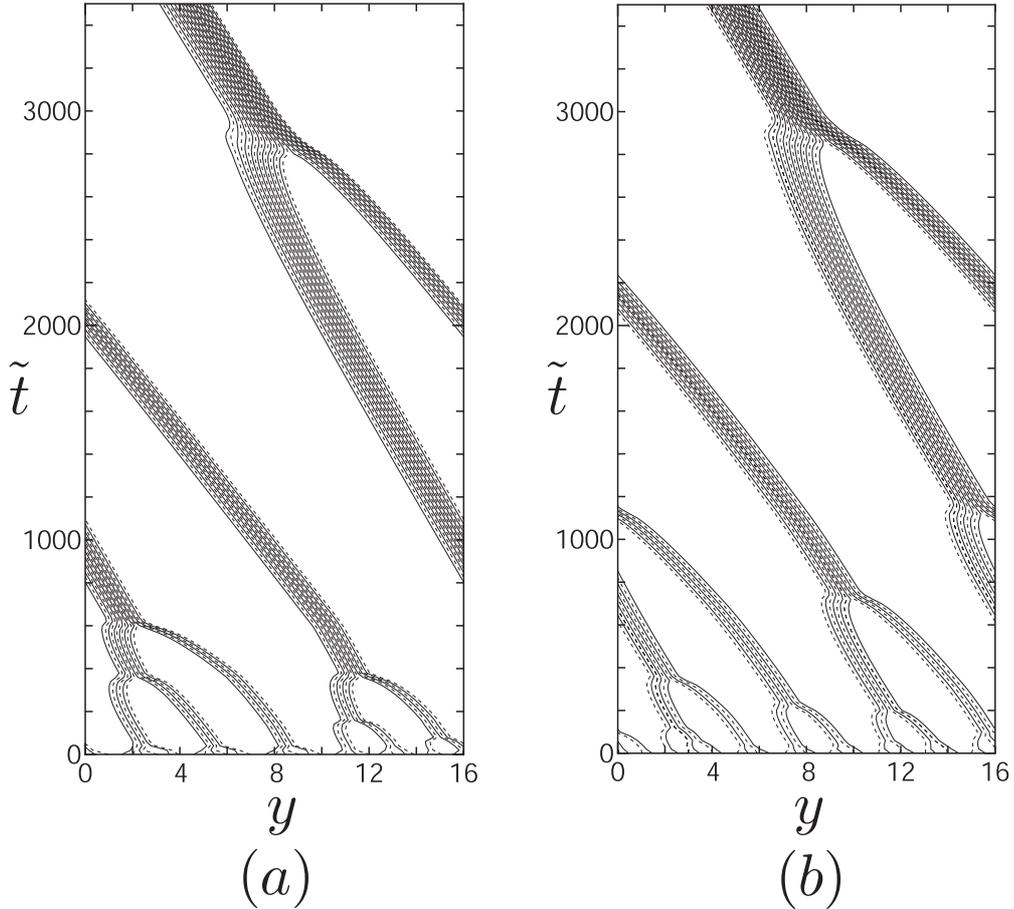
FIG. 7: Time evolution of step positions in sublimation with (a) step-down drift and (b) step-up drift. Parameters are $f = 0.2$, $D_{\mathrm{B}} = 2$, $D_{\mathrm{A}} = 1$, $\tilde{A}_2 = 10^{-4}$ with $\nu = 2$ and the lifetime $\tau = 80$. The number of steps is 32 and the initial step distance is 0.5.

The above effect of evaporation is also seen in the exponent β. Figure 8 shows the bunch size as a function of time. The data are obtained in the same way as in Fig. 6. In a later stage, the step bunches grow as $N \sim t^\beta$. The exponent is about $\beta \approx 0.55$ with step-down drift and $\beta \approx 0.75$ with step-up drift. These values are larger than those without evaporation.

With increasing the evaporation rate, the growth process changes drastically. Figure 9 represents the time evolution of step positions for a large evaporation rate. The pairing of steps occurs in the initial stage. With step-up drift (Fig.9(b)), only small bunches and step pairs are seen. The bunches repeat collisions with isolated step pairs and the bunch size is saturated. With step-down drift (Fig. 9(a)), a large bunch appears and collides with a step pair in a later stage. With further increase of the evaporation rate, the motion of steps with step-down drift becomes similar to that with step-up drift. These features are similar to the

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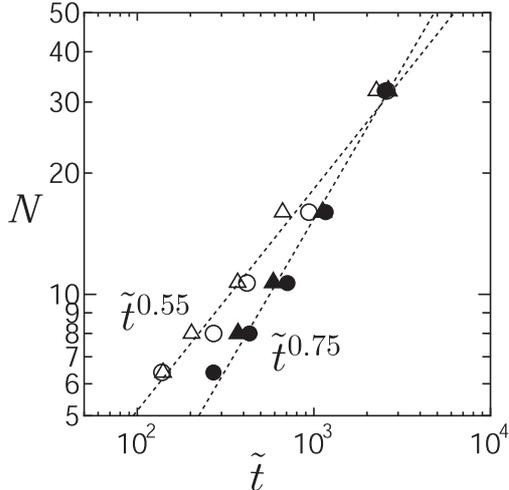
FIG. 8: Time dependence of bunch size in sublimation with the potential of $\nu = 0$ and of $\nu = 2$. The parameters are the same as in Fig. 7 for $\nu = 2$. For $\nu = 0$, $\tilde{A}_0 = 10^{-2}$ and other parameters are the same as in Fig. 7. The open marks indicate step-down drift ($\triangle$ $\nu = 0$ and $\bigcirc$ $\nu = 2$), and filled marks indicate step-up drift.

case of bunching on a simple vicinal face [12].

IV. SUMMARY AND DISCUSSION

By the use of a one-dimensional step model we studied the growth laws in the drift-induced step bunching on a vicinal face of Si(001) with alternating diffusion coefficient. In contrast to the case of Si(111) [12], the step bunching occurs both with step-up and step-down drift. The origin of step pairing with drift in both directions is simple and evident, but the formation of large bunches in both drift directions was surprising at first.

The reason of the difference between Si(111) and Si(001) is the following. If a bunch is formed out of repulsive steps, the force acting on the upper edge step is negative (*i.e.* to the left direction) and that on the lower edge step is positive (to the right). In terms of equilibrium adatom density, this means that the density is high at the left and low at the right edge of the bunch. For the step bunch to be stable against dissociation, the density profile on the large terrace must be consistent with these values. This is attained by the density distribution, which has the form $c(y) = c_1 + c_2 e^{fy}$, in both drift directions if $c_2 f > 0$. The density change in the bunch is achieved by the difference of the diffusion coefficient as

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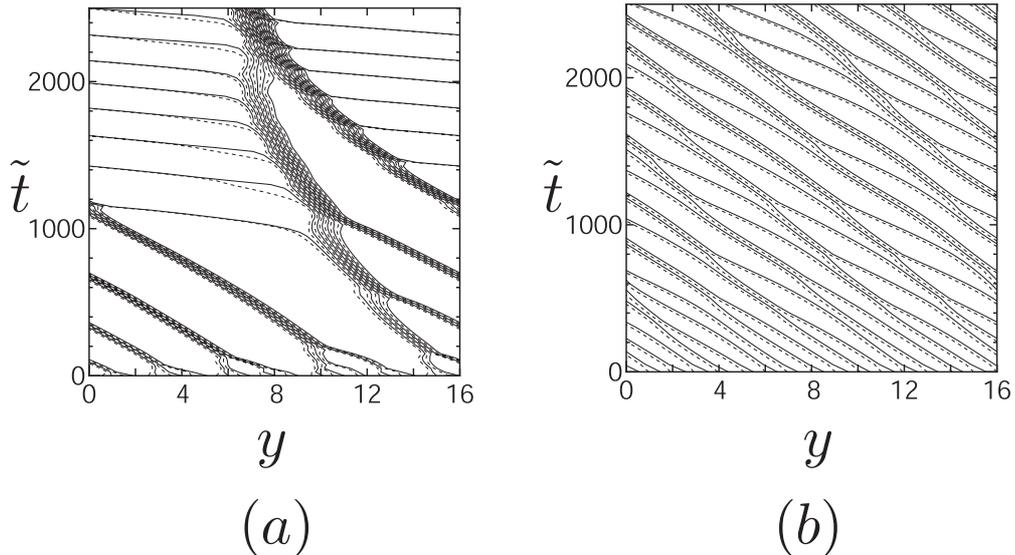
FIG. 9: Time evolution of step positions with a large evaporation rate with (a) step-down drift and (b) step-up drift. Parameters are $|f| = 0.1$, $D_B = 1$, $D_A = 0.1$, $\tilde{A}_2 = 10^{-4}$ with $\nu = 2$ and the lifetime $\tau = 50$. The number of steps is 32.

seen in Fig.4.

In contrast, on Si(111) the density change occurs at the steps and is due to the kinetic barrier for solidification (finiteness of the kinetic coefficient). The gradient of the adatom density on terraces in the bunch is small. When the drift is in the step-down direction, adatoms are incorporated to the bunch from the left and released from the right edge, and the step bunch is stable. With the step-up drift, the adatoms are incorporated to the bunch from the right and released from the left edge. Then the adatom density at the right edge of the bunch should be higher than that at the left, which is not consistent with the equilibrium adatom density at the steps. Thus the formation of a bunch with step-up drift is not possible on Si(111). In both systems, once the stable bunch is formed, the coalescence of bunches proceed in the same way.

The growth rate of bunch size with step-down drift is faster than that with step-up drift. The average step distance l_b in the bunch becomes small with the increase of the bunch size as $l_b \sim N^{-\alpha}$. The exponents α obtained by the simulation fit the simple formula $\alpha = 3/2(\nu+2)$, where ν is the power of the repulsive potential between steps. In a conserved system the bunch size N increases with time t as $N \sim t^\beta$. In contrast to the case of standard drift-induced bunching [12], the exponent β is weakly dependent on ν. The exponent α and

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β are related as $\beta = 1/(2 + \alpha)$.

In the experiment [2], the bunch size increases as $N \sim t^\beta$ with $\beta \approx 1/2$, and the growth rate with step-up drift is about the same as that with step-down drift. In our numerical simulation, the exponent β in the conserved system is slightly smaller than that in the experiment, and the growth rate changes with the drift direction (Fig. 6). The difference of the growth rate is as large as that of the two diffusion coefficients. Since the experiment [2] was carried out at high temperature, the evaporation may not be negligible. In our simulation, the difference of growth rate decreases as the evaporation increases. However, the exponent β is larger than that in a conserved system and depends on the drift direction. In the previous studies [19–21], the ratio of the two diffusion coefficients are estimated to be $2 \sim 1000$. Although the evaporation may have an important effect, the disagreement between the experiment and the simulation is not resolved only by the evaporation.

On a Si(001) vicinal face, the step-step interaction potential is logarithmic repulsion [17]. The average step distance l_b in a bunch decreases as $l_b \sim N^{-\alpha}$ with $\alpha = 0.5$ in the experiment [2]. In our simulation with logarithmic interaction potential, the exponent is $\alpha \approx 0.75$. In addition to the logarithmic potential between steps, which originates from the inequivalent terraces, there must be a $1/l^2$ potential due to the force dipole at the step [22, 23]. The $1/l^2$ potential is important when the step distance becomes small in a tight bunch. Since the exponent α is 0.38 for the repulsive potential $\nu = 2$, we tried a potential $\zeta = -A_0 \ln l + A_2/l^2$. Then the exponent $\alpha \approx 0.5$ and $\beta \approx 0.4$ are reproduced as shown in Figs. 10(a) and (b), respectively. The relation between α and β expected from eq. (18) is satisfied.

In the simulation, the step distance l_b in a bunch is $l_b \sim 10^{-2}$ when the step number is $N \approx 10$. The ratio of the two repulsive forces derived from $A_0 \ln l$ and A_2/l^2 is of the order of unity: $A_0 l_b^{-2}/A_2 l_b^{-4} \sim \mathcal{O}(1)$. On a Si(001) vicinal face, the coefficient A_0 was estimated as $A_0 \approx 0.003 \,\text{eV/Å}$ [17]. In the experiment [2], which was carried out at $T \sim 1150-1170°\text{C}$, the step distance is $l_b \approx 2\text{nm}$ when the step number is $N \approx 10$. The coefficient A_2 is estimated to be $A_2 = A_0 l_b^2 \approx 0.12$ eV nm. This value A_2 for Si(001) is as large as the estimated repulsion strength on a Si(111) vicinal face: $A_2^{(111)} \approx 0.17$ eV nm at $T \approx 1160°\text{C}$ [16]. Since the origin of the dipole repulsion is in common, the estimated order of magnitude of A_2 is reasonable. Thus the experimental value of α is an indication that both the logarithmic potential and the dipole potential are important in the step bunch.

Our simple model with alternating diffusion anisotropy gives a good account for the step
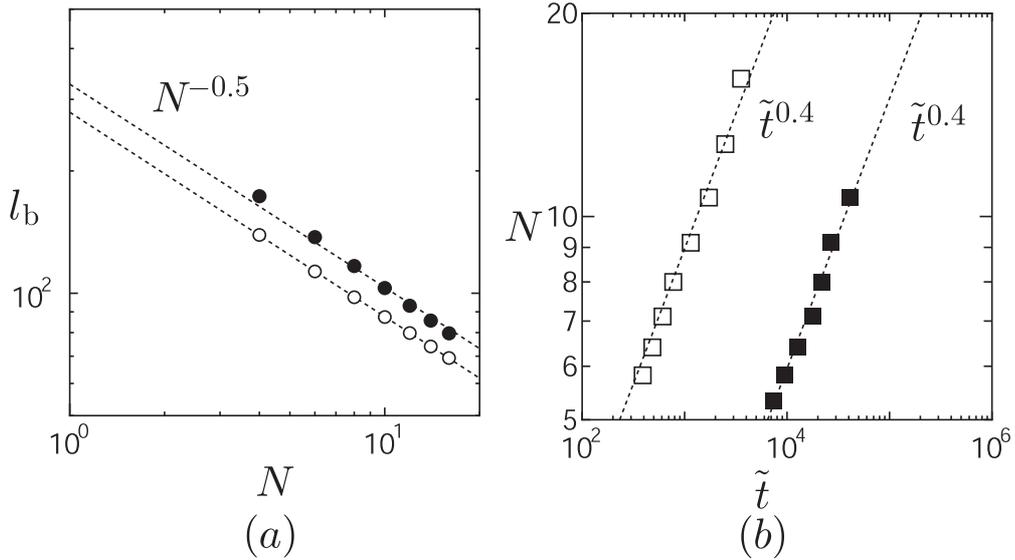
FIG. 10: (a)Dependence of the step distance l_b on the bunch size N and (b) time dependence of N. The open marks are for step-down drift and the filled marks are for step-up drift. The repulsive potential is $\zeta = -A_0 \ln l + A_2/l^2$ with $A_0 = 5.0 \times 10^{-4}$ and $A_2 = 5.0 \times 10^{-8}$ for step-down drift and $A_0 = 2.0 \times 10^{-4}$ and $A_2 = 2.0 \times 10^{-8}$ for step-up drift. Other parameters are $D_A = 1.0$, $D_B = 0.1$ and $f = 1.0$ (a), $f = 0.1$ (b).

bunching as well as the step wandering [24, 25] instabilities on Si(001). However, there are two disagreements between our simulation and the experiment [2]. In our simulation, the average width l_b with the step-up drift is larger than that with the step-down drift if the parameters are the same, which is the opposite to the experiment [2]. Also in our simulation the bunches with step-down drift grows faster than that with step-up drift contrary to the experiment. We think the latter problem is rather serious and further study is needed.

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