Evaporation and impingement effects on drift-induced step instabilities on a Si(001) vicinal face

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(Received 31 January 2005; published 1 July 2005)

We theoretically study the effect of evaporation and impingement of atoms on step wandering induced by the drift of adatoms. With a Si(001) vicinal face in mind, the anisotropy in diffusion coefficient is assumed to alternate on consecutive terraces. Without evaporation, steps wander in-phase with step-up drift and grooves perpendicular to the steps appear. The form of the wandering steps is sinusoidal with the width increasing in time as $t^{1/2}$. Evaporation of adatoms suppresses the step wandering and introduces two surface diffusion lengths. When they are longer than the step distance, the step width still increases in proportion to $t^{1/2}$, but with a smaller coefficient than that in the case without evaporation. When one of the surface diffusion lengths is comparable or shorter than the step distance, the saturation of the step width occurs. Impingement of atoms, on the other hand, changes the form of the wandering steps: their front becomes flat and wide and the grooves become steep and narrow. The growth rate of the step width becomes small, but the step width increases with the same exponent 1/2.

DOI: 10.1103/PhysRevB.72.045401 PACS number(s): 81.10.Aj, 05.70.Ln, 47.20.Hw, 68.35.Fx

I. INTRODUCTION

The Si(001) surface is reconstructed by the dimerization of surface atoms. When a vicinal face is tilted in the $\langle 110 \rangle$ direction, T_A terraces, where the dimer rows are parallel to the steps, and T_B terraces, where the dimer rows are perpendicular to the steps, appear alternately. Since the surface diffusion along the dimer rows is faster than that perpendicular to the dimer rows,[1] the direction of the fast surface diffusion changes on consecutive terraces.

Nielsen and co-workers[2] observed steps on the vicinal face heated by direct electric current. When the current is in the step-down direction, step bunching occurs. When the current is in the step-up direction, the step bunching occurs on a region of small inclination. With increasing the inclination (about 0.08–0.5°), the step bunching is suppressed and in-phase step wandering occurs. Straight grooves parallel to the current appear on the vicinal face.

The step wandering is caused by the drift of adatoms induced by the current. With taking account of the alternation of the anisotropy of surface diffusion, we have theoretically studied[3] the step wandering induced by the drift. If the step-step repulsion is weak, the step bunching occurs irrespective of the drift direction. With a strong step repulsion, the step bunching is suppressed and the in-phase step wandering occurs with step-up drift. Since the step repulsion is strong for the large inclination, our results has the same tendency with the experiment.[2]

In the previous analysis,[3] we neglected the evaporation and impingement of atoms. However, the experiment[2] was carried out at a high temperature, and the evaporation may be important. On the Si(001) vicinal face, the observation during growth has not yet been attempted, but it is probably possible as on a Si(111) vicinal face.[4]

In this paper, we study effect of the evaporation and the impingement on the drift-induced step wandering. In Sec. II, we introduce a step flow model. We study the effect of evaporation in Sec. III and impingement in Sec. IV. We carry out a linear stability analysis to find the condition for the step wandering, and a Monte Carlo simulation to see the behavior of the unstable steps. In Sec. V, we summarize the results with a brief discussion.

II. MODEL

For the stability analysis we use a step flow model,[3,5–14] in which the step velocity is determined by the mass conservation at step positions. We assume that the steps are parallel to x axis on average, and the slope is downward in the positive y direction. The diffusion equation of the adatom density $c(\boldsymbol{r},t)$ is given by

$$\frac{\partial c(\boldsymbol{r},t)}{\partial t} = -\nabla \cdot \boldsymbol{j}(\boldsymbol{r},t) - \frac{1}{\tau} c(\boldsymbol{r},t) + F_{\mathrm{im}}, \tag{1}$$

where $\boldsymbol{j}(\boldsymbol{r},t)$ is the adatom current on the surface, τ the lifetime of adatoms for evaporation and F_{im} is the impingement rate of atoms from the vapor phase. The current is given by

$$\boldsymbol{j}(\boldsymbol{r},t) = -\left(D_x \frac{\partial c}{\partial x} \hat{\boldsymbol{e}}_x + D_y \frac{\partial c}{\partial y} \hat{\boldsymbol{e}}_y \right) + D_y \frac{Fc}{k_B T} \hat{\boldsymbol{e}}_y, \tag{2}$$

where $\hat{\boldsymbol{e}}_x$ and $\hat{\boldsymbol{e}}_y$ are the unit vectors in the x and y directions. The first term in Eq. (2) represents the surface diffusion and the second term represents the drift of adatoms. F is the force to induce the drift. The diffusion coefficient $D_\perp$ perpendicular to the dimers, is larger than that $D_\parallel$ parallel to the dimers. The diffusion coefficients are $(D_x, D_y) = (D_\parallel, D_\perp)$ on T_B terraces, and $(D_x, D_y) = (D_\perp, D_\parallel)$ on T_A terraces (Fig. 1).

In our previous study,[14] the growth law of the step bunching for the model with infinite kinetic coefficient agrees with the experiment.[15] In the limit of fast kinetics, the adatom density at the steps is in equilibrium with the steps

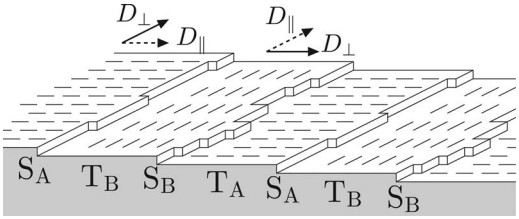

FIG. 1. A Si(001) vicinal face tilted in ⟨110⟩ direction. Short lines on the terraces represent dimers.

$$c|_\zeta = c_{\rm eq}^0\left[1+\frac{\Omega\tilde{\beta}\kappa}{k_{\rm B}T}+\frac{\Omega}{k_{\rm B}T}\frac{\partial}{\partial y}[U(l_+)+U(l_-)]\right], \tag{3}$$

where $y=\zeta(x,t)$ is the step position, $c_{\rm eq}^0$ the equilibrium adatom density for an isolated straight step, Ω the atomic area, $\tilde{\beta}$ the step stiffness and κ the curvature of the step. U is the step-step interaction potential. $l_{+(-)}$ is the terrace width of the lower (upper) side terrace. We assume that the step interaction is present only between neighboring steps and the form of the interaction potential is $U(l)=A/l^n$ or $U(l)=A\ln l$.[16]

By solving the diffusion equation (1) in the quasistatic approximation ($\partial c/\partial t=0$) with the boundary condition (3), the adatom density is determined. The step velocity is

$$V=\Omega\hat{\boldsymbol{n}}\cdot(\boldsymbol{j}|_{\zeta+}-\boldsymbol{j}|_{\zeta-}), \tag{4}$$

where $\boldsymbol{j}$ is given by Eq. (2).

III. EFFECT OF EVAPORATION

A. Linear stability analysis

Without evaporation, in-phase step wandering occurs with step-up drift.[14] In this section, we study effect of the evaporation on the step wandering without impingement of atoms. On the vicinal face with the step distance l, the velocities $V_{\rm A}$ of step $S_{\rm A}$ and $V_{\rm B}$ of $S_{\rm B}$ are given by

$$V_A=\Omega D_\perp c_{\rm eq}^0\left(-\frac{f}{2}-\Lambda_\perp\frac{\cosh\Lambda_\perp l-e^{-fl/2}}{\sinh\Lambda_\perp l}\right)-\Omega D_\parallel c_{\rm eq}^0\left(-\frac{f}{2}+\Lambda_\parallel\frac{\cosh\Lambda_\parallel l-e^{-fl/2}}{\sinh\Lambda_\parallel l}\right), \tag{5}$$

$$V_B=\Omega D_\parallel c_{\rm eq}^0\left(-\frac{f}{2}-\Lambda_\parallel\frac{\cosh\Lambda_\parallel l-e^{-fl/2}}{\sinh\Lambda_\parallel l}\right)-\Omega D_\perp c_{\rm eq}^0\left(-\frac{f}{2}+\Lambda_\perp\frac{\cosh\Lambda_\perp l-e^{-fl/2}}{\sinh\Lambda_\perp l}\right). \tag{6}$$

In Eqs. (5) and (6), the parameters, f, $\Lambda_\perp$ and $\Lambda_\parallel$ are defined as

$$f=\frac{F}{k_{\rm B}T}, \tag{7}$$

$$\Lambda_\perp=\frac{1}{2}\sqrt{f^2+\frac{4}{x_\perp^2}}, \tag{8}$$

$$\Lambda_\parallel=\frac{1}{2}\sqrt{f^2+\frac{4}{x_\parallel^2}}, \tag{9}$$

where $x_\perp=\sqrt{D_\perp\tau}$ is the surface diffusion length along the dimer rows, and $x_\parallel=\sqrt{D_\parallel\tau}$ is that perpendicular to the dimer rows. When the terrace width is small such that $\Lambda_\perp l\ll 1$ and $\Lambda_\parallel l\ll 1$, the step velocities $V_{\rm A}$ and $V_{\rm B}$ are approximated as

$$V_{\rm A}=\Omega c_{\rm eq}^0\left[-\frac{l}{\tau}-(D_\perp-D_\parallel)f\right], \tag{10}$$

$$V_{\rm B}=\Omega c_{\rm eq}^0\left[-\frac{l}{\tau}+(D_\perp-D_\parallel)f\right]. \tag{11}$$

In Eqs. (10) and (11), the first terms proportional to the evaporation rate are always negative: the steps recede by the evaporation. Since the contribution of the evaporation to $V_{\rm A}$ and $V_{\rm B}$ are the same, the evaporation does not cause step pairing. The second terms proportional to the drift velocity vanish if the surface diffusion is isotropic. If the drift is in the step-down direction ($f>0$), the second term in Eq. (10) is negative and that in Eq. (11) is positive. $S_{\rm A}$ steps recede faster than $S_{\rm B}$, and step pairs separated by large $T_{\rm B}$ terraces appear. When the drift direction is the opposite ($f<0$), step pairs separated by $T_{\rm A}$ terraces appear.

If step distances alternate $l_{\rm A}$ and $l_{\rm B}$ consecutively, the equilibrium adatom density $c_{\rm A}$ of $S_{\rm A}$ is different from $c_{\rm B}$ of $S_{\rm B}$ due to the repulsive interaction. From the condition that the steps move at the same velocity, $V_{\rm A}=V_{\rm B}$, the difference of the equilibrium adatom density $\Delta c=c_{\rm B}-c_{\rm A}$ is determined as

$$\frac{\Delta c}{2c_{\rm eq}^0}=\frac{D_\perp}{v}\left(\Lambda_\perp\frac{\sinh fl_{\rm B}/2}{\sinh\Lambda_\perp l_{\rm B}}+\frac{f}{2}\right)-\frac{D_\parallel}{v}\left(\Lambda_\parallel\frac{\sinh fl_{\rm A}/2}{\sinh\Lambda_\perp l_{\rm A}}+\frac{f}{2}\right), \tag{12}$$

where $l_{\rm A}$ is the width of $T_{\rm A}$, $l_{\rm B}$ that of $T_{\rm B}$, and v is defined as

$$v=\frac{D_\perp\Lambda_\perp}{\sinh\Lambda_\perp l_{\rm B}}(\cosh fl_{\rm B}+\cosh\Lambda_\perp l_{\rm B})+\frac{D_\parallel\Lambda_\parallel}{\sinh\Lambda_\parallel l_{\rm A}}(\cosh fl_{\rm A}+\cosh\Lambda_\parallel l_{\rm A}). \tag{13}$$

When the difference of the terrace width ($\Delta l=l_{\rm B}-l_{\rm A}$) is small, Δc is approximately written as $\Delta c=\Delta c_0+\Delta c_1$ with

$$\Delta c_0=\frac{(D_\perp-D_\parallel)}{(D_\perp+D_\parallel)}\frac{Flc_{\rm eq}^0}{k_{\rm B}T}, \tag{14}$$

$$\Delta c_1=-\frac{l^2\Delta c_0}{6(D_\perp+D_\parallel)\tau}, \tag{15}$$

where we have assumed $(fx_\perp)^2\ll 1$, $(fx_\parallel)^2\ll 1$, $(fl)^2\ll 1$ and $\Delta l/l\ll 1$.

Δc_0 is the difference of the equilibrium adatom density without evaporation.[3] Δc_1 is due to the evaporation and suppresses the effect of Δc_0. From the step-step repulsion, Δc is expressed as

$$\Delta c = \frac{2\Omega c_{\rm eq}^0}{k_{\rm B}T}[U'(l_{\rm B}) - U'(l_{\rm A})] \approx g\Delta l, \tag{16}$$

where g is given by

$$g = -\frac{2\Omega c_{\rm eq}^0}{k_{\rm B}T}\frac{d^2U}{dl^2} = -\frac{2n(n+1)A\Omega c_{\rm eq}^0}{k_{\rm B}Tl^{n+2}}. \tag{17}$$

From Eqs. (14)–(16), the difference of the terrace width is determined by

$$\frac{\Delta l}{l} = -\frac{Fc_{\rm eq}^0(D_\perp - D_\parallel)}{g(D_\parallel + D_\perp)k_{\rm B}T}\left[1 - \frac{l^2}{6(D_\perp + D_\parallel)\tau}\right]. \tag{18}$$

If the step distance is shorter than the surface diffusion length, $l \ll x_\perp$, the second term is neglected.

We give small fluctuations, $\zeta_{\rm A}e^{iqx}$ to straight S_A steps and $\zeta_{\rm B}e^{iqx}$ to straight S_B steps. Evolution of the fluctuations is expressed as

$$\frac{d\zeta_{\rm A}}{dt} = \mathcal{F}_{\rm A}^{(D)} + \mathcal{F}_{\rm A}^{(\tilde{\beta})} + \mathcal{F}_{\rm A}^{(U)}, \tag{19}$$

$$\frac{d\zeta_{\rm B}}{dt} = \mathcal{F}_{\rm B}^{(D)} + \mathcal{F}_{\rm B}^{(\tilde{\beta})} + \mathcal{F}_{\rm B}^{(U)}, \tag{20}$$

where $\mathcal{F}$s are given in Appendix A. In Eqs. (19) and (20), the second terms proportional to the step stiffness suppress the step wandering, and the third terms proportional to g suppress step bunching (the fluctuation of the step distance). The first terms may destabilize the straight steps.

If the step distance is small so that the repulsion is strong, Eqs. (19) and (20) are expanded up to the first order correction in l, and the evolution equations are approximately given by

$$\frac{d\zeta_A}{dt} = -\frac{d\zeta_B}{dt} = \frac{\Omega\Delta c_0}{l^2}(D_\perp - D_\parallel)(\zeta_{\rm A} - \zeta_{\rm B}) - \frac{\Omega(\Gamma + 2g)}{l}(D_\perp + D_\parallel)(\zeta_{\rm A} - \zeta_{\rm B}), \tag{21}$$

where $\Gamma = \Omega\tilde{\beta}/k_{\rm B}T$. The effect of evaporation does not appear in this order. The amplitude of the fluctuations increases as $\zeta_{\rm A}, \zeta_{\rm B} \sim e^{\omega t}$ with the rate ω, which is given by

$$\omega_{\rm out} = 2\Omega\frac{\Delta c_0}{l^2}(D_\perp - D_\parallel) - 2\Omega\frac{(\Gamma + 2g)}{l}(D_\perp + D_\parallel), \tag{22}$$

$$\omega_{\rm in} = 0. \tag{23}$$

The subscripts indicate out-of-phase fluctuation, $\zeta_{\rm A} = -\zeta_{\rm B}$, and in-phase fluctuation, $\zeta_{\rm A} = \zeta_{\rm B}$. From Eq. (16), the first term of $\omega_{\rm out}$ is smaller than the second term, and the out-of-phase fluctuation decays irrespective of the drift direction. The amplification rate $\omega_{\rm in}$ vanishes and the steps are marginal to the in-phase fluctuation. If we expand Eqs. (19) and (20) up to the third order in l, $\omega_{\rm in}$ is given by

$$\omega_{\rm in} = -\frac{\Omega(D_\perp - D_\parallel)\Delta c}{2}q^2 - \frac{\Omega(D_\parallel + D_\perp)l}{2}\Gamma q^4, \tag{24}$$

where we have assumed $\Gamma f/\Delta c \ll 1$. With step-down drift, the first term is negative and the step wandering does not occur. With step-up drift, the first term is positive and the steps are unstable to a long wavelength fluctuation. The wavelength of the most unstable mode, $\lambda_{\rm max}$ is given by

$$\lambda_{\rm max} = 2\pi\sqrt{\frac{2\Gamma(D_\perp + D_\parallel)l}{(D_\parallel - D_\perp)\Delta c}}, \tag{25}$$

and the amplification rate of the most unstable mode, $\omega_{\rm max}$ is

$$\omega_{\rm max} = \frac{[(D_\perp - D_\parallel)\Delta c]^2}{8c_{\rm eq}^0(D_\perp + D_\parallel)l\Gamma}. \tag{26}$$

Equation (24) has the same form as the amplification rate in the conserved system with the replacement of Δc_0 by Δc. The effect of evaporation appears only in Δc. The wavelength $\lambda_{\rm max}$ increases and the amplification rate $\omega_{\rm max}$ decreases with increasing evaporation. Thus the evaporation stabilizes the vicinal face.

B. Monte Carlo simulation

From the linear analysis, we found the condition for the step wandering. To study the behavior of unstable steps, we carry out Monte Carlo simulation.[3,10,13,17] We use a square lattice model with the lattice constant $a=1$. 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: step positions are single-valued functions of x. The time increment for a diffusion trial is set $\Delta t = 1/4N_a$ (N_a is the number of adatoms) so that the larger diffusion coefficient is $D_\perp = 1$. Long-range step repulsion is taken into account in the y direction. In the x direction, only the short range repulsion is taken account by forbidding overlap of steps.

During the time interval Δt, an adatom evaporates with the probability $\Delta t/\tau$. On T_A terraces, an adatom at the site (i,j) moves to $(i\pm1,j)$ with the probability 1/4 and to $(i,j\pm1)$ with the probability $p_{\rm d}(1 \pm Fa/2k_{\rm B}T)/4$, where F is the external force to induce the drift and $p_{\rm d} = D_\parallel/D_\perp (\leqslant 1)$ represents the strength of the anisotropy of the diffusion. On T_B terraces, an adatom at the site (i,j) moves to $(i\pm1,j)$ with the probability $p_{\rm d}/4$ and to $(i,j\pm1)$ with the probability $(1 \pm Fa/2k_{\rm B}T)/4$. In the simulation we use the permeable steps:[13] adatoms diffuse over steps to the neighboring terraces without an extra potential barrier. The diffusion between neighboring terraces is assumed to occur with the transition probability of the upper side terrace.

When an adatom comes in contact with a step from the lower terrace, solidification occurs with the probability

$$p_{\rm s} = \left[1 + \exp\left(\frac{\Delta E_s + \Delta U - \phi}{k_{\rm B}T}\right)\right]^{-1}. \tag{27}$$

When there is no adatom on top of a solid atom at the step position, melting of the solid atom occurs with the probability

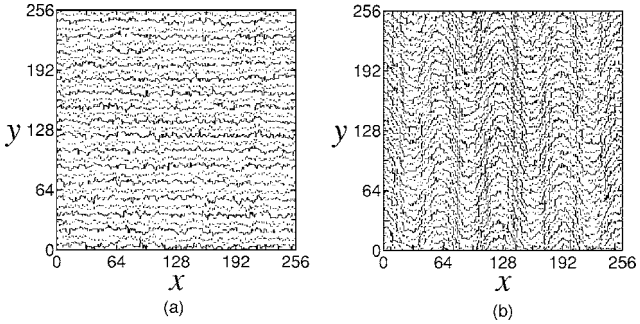

FIG. 2. Snapshots of the step wandering without evaporation: (a) with step-down drift $f=0.05$ at $t=5.0\times10^5$ and (b) with step-up drift $f=-0.05$ at $t=5.0\times10^5$.

$$p_{\mathrm{m}}=\left[1+\exp\left(\frac{\Delta E_{\mathrm{s}}+\Delta U+\phi}{k_{\mathrm{B}}T}\right)\right]^{-1}. \tag{28}$$

ΔE_s is the increment of the step energy and ϕ the energy gain by solidification. ΔE_s is given by $\Delta E_s=\epsilon\times$ (the increment of the step perimeter), where the half of the nearest-neighbor bond energy, ϵ, is related to the step stiffness $\tilde{\beta}$ as

$$\frac{2\tilde{\beta}}{k_{\mathrm{B}}T}=\sinh^2\frac{\epsilon}{2K_{\mathrm{B}}T}. \tag{29}$$

The equilibrium adatom density of an isolated step, c_{eq}^0 satisfies the detailed balance $c_{\mathrm{eq}}^0 p_{\mathrm{s}}=(1-c_{\mathrm{eq}}^0)p_{\mathrm{m}}$ at kink sites. Since the perimeter length does not change by solidification or by melting at the kink sites, the change of the step energy vanishes, and c_{eq}^0 is given by[17]

$$c_{\mathrm{eq}}^0=\frac{1}{1+e^{\phi/k_{\mathrm{B}}T}}. \tag{30}$$

ΔU is the change of step-step interaction potential. On a Si(001) vicinal face, the repulsive interaction potential between straight steps is logarithm of the terrace width.[16] For the long-range interaction potential between the nth and the $(n+1)$th steps, we use

$$U=\sum_{x_i}A\ln|y_n(x_i)-y_{n+1}(x_i)|, \tag{31}$$

where $y_n(x_i)$ is the y coordinate of the nth step at $x=x_i$.

We first carry out the simulation without evaporation. Figure 2 shows the motion of steps without evaporation. Solid lines represent S_B steps and dotted lines represent S_A steps. At the beginning, all the steps are straight with the step distance $l=8$, and only a few adatoms are present on the terraces. The system size is 256×256 and the number of steps is 32. The parameters are so chosen as the equilibrium adatom density is $c_{\mathrm{eq}}^0=0.18$, the step stiffness is $\tilde{\beta}/k_{\mathrm{B}}T=0.13$. The diffusion coefficients are $D_{\parallel}=0.5$ and $D_{\perp}=1.0$. The kinetic coefficient is so large that the local equilibrium condition at the steps is valid. The strength of repulsive potential is $A/k_{\mathrm{B}}T=4.6$ and strong enough to suppress step bunching. When the drift is in the step-down direction with $f=0.05$, the step wandering does not occur and the steps are straight [Fig. 2(a)]. The step wandering occurs when the drift is in the step-up direction with $f=-0.05$ [Fig. 2(b)]. The results agree with the linear analysis.[3,8,10–12] Because of the in-phase step wandering, hills and valleys parallel to the y axis appear periodically. The formation of straight grooves is explained by the nonlinear analysis.[3,8,11] The form of wandering steps is sinusoidal and symmetric in the y direction.

Figure 3 shows the wandering of steps with evaporation. In Fig. 3(a), the lifetime of adatoms is $\tau=512$. The shorter surface diffusion length is $x_{\parallel}=16$, which is twice as long as the initial step distance. The effect of the evaporation is small: the width and the form of grooves are similar to that of Fig. 2(b). In Fig. 3(b), the lifetime is $\tau=256$ and the surface diffusion length $x_{\parallel}=8\sqrt{2}$ is longer than the step distance. The width of grooves becomes wider than that without evaporation, but the form of grooves is similar to Fig. 3(a). In Fig. 3(c), the lifetime is $\tau=128$ and $x_{\parallel}=8$ is as long as the step distance. The wavelength of the grooves becomes longer and the growth of the amplitude is slow. These features qualitatively agree with the linear analysis.

When the surface diffusion lengths are longer than the step distance, the form of the wandering steps is sinusoidal and symmetric in the y direction as in the conserved system. The form becomes asymmetric when the surface diffusion length becomes comparable or shorter than the step distance. The hills are narrower than the valleys. The asymmetry may be caused by the same nonlinear effect as in the KPZ equation. The evaporation also changes the growth law of step width, which is defined as

$$w(t)=\frac{1}{N}\sum_{n=1}^{N}\sqrt{\frac{1}{L}\sum_{i=1}^{L}\left[y_n(i)-\frac{1}{L}\sum_{i}^{L}y_n(i)\right]^2}. \tag{32}$$

N is the number of steps and L the system size in the x direction. Figure 4 shows the time evolution of the amplitude w for several evaporation rates. The results are obtained by

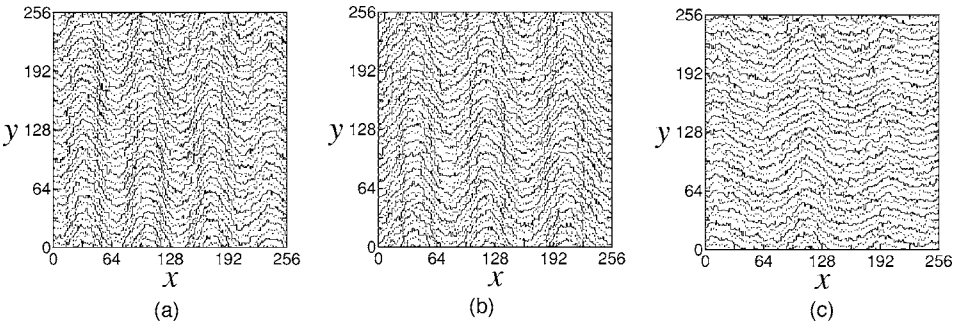

FIG. 3. Snapshots of the step wandering during sublimation with step-up drift $f=-0.05$ at $t\approx5.0\times10^5$. The lifetime of adatoms is (a) $\tau=512$, (b) $\tau=256$, and (c) $\tau=128$.

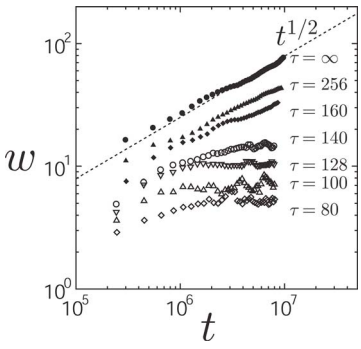

FIG. 4. Time evolution of the step width with several evaporation rate.

averaging over 10 runs of the size 512×128 with 16 steps. In the conserved system, the step width increases rapidly in an early stage. In a late stage the width increases as $w\sim t^{\beta}$ with $\beta\approx1/2$.[3,8,11,12] When the evaporation rate is small, the rapid growth of the step width in an early stage is similar to that in the conserved system. When the evaporation rate is so large and the short diffusion length is as long as or shorter than the step distance, the step width is saturated in a late stage.

IV. EFFECT OF IMPINGEMENT

A. Linear stability analysis

In this section, we study the effect of the impingement of adatoms on the step wandering. To focus on the impingement of adatoms, we neglect the evaporation. When the steps are straight and equidistant with a separation l, the velocities of steps are given by

$$V_{\mathrm{A}}=\Omega[F_{\mathrm{im}}l+(D_{\perp}-D_{\parallel})fc_{\mathrm{eq}}^{0}], \tag{33}$$

$$V_{\mathrm{B}}=\Omega[F_{\mathrm{im}}l-(D_{\perp}-D_{\parallel})fc_{\mathrm{eq}}^{0}]. \tag{34}$$

Since the contribution of the impingement to S_{A} is the same as to S_{B}, the impingement does not cause the step pairing. The step pairing is induced by the second terms in Eqs. (33) and (34), which is proportional to the product of the difference of the diffusion coefficients and the drift of adatoms. The step distance in a pair is determined by the condition $V_{\mathrm{A}}=V_{\mathrm{B}}$. When steps are paired with alternating distances l_{A} and l_{B}, the condition is

$$\begin{aligned}\left(D_{\perp}\tanh\frac{fl_{\mathrm{A}}}{2}-D_{\parallel}\tanh\frac{fl_{\mathrm{B}}}{2}\right)f\Delta c&=F_{\mathrm{im}}\left(l_{\mathrm{B}}\tanh\frac{fl_{\mathrm{A}}}{2}-l_{\mathrm{A}}\tanh\frac{fl_{\mathrm{B}}}{2}\right)\\&\quad+2fc_{\mathrm{eq}}^{0}(D_{\perp}-D_{\parallel})\tanh\frac{fl_{\mathrm{A}}}{2}\tanh\frac{fl_{\mathrm{B}}}{2}.\end{aligned} \tag{35}$$

If the step distance is small $fl_{\mathrm{A}},fl_{\mathrm{B}}\ll1$, the first term of the right-hand side of Eq. (35) is of the order of $F_{\mathrm{im}}f^{3}l^{3}\Delta l$ and the second term is $\sim c_{\mathrm{eq}}^{0}Df^{3}l^{2}$. As long as the impingement is weak $F_{\mathrm{im}}\ll c_{\mathrm{eq}}^{0}D/l\Delta l$, the effect on Δc is negligible.

To study the step wandering on the vicinal face, we give small fluctuations $\zeta_{\mathrm{A}}(t)e^{iqx}$ to $\mathrm{S_A}$ and $\zeta_{\mathrm{B}}(t)e^{iqx}$ to $\mathrm{S_B}$. The linearized evolution equations are given by

$$\frac{d\zeta_{\mathrm{A}}}{dt}=\mathcal{G}_{\mathrm{A}}^{(D)}+\mathcal{G}_{\mathrm{A}}^{(F_{\mathrm{im}})}+\mathcal{G}_{\mathrm{A}}^{(\tilde{\beta})}+\mathcal{G}_{\mathrm{A}}^{(U)}, \tag{36}$$

$$\frac{d\zeta_{\mathrm{B}}}{dt}=\mathcal{G}_{\mathrm{B}}^{(D)}+\mathcal{G}_{\mathrm{B}}^{(F_{\mathrm{im}})}+\mathcal{G}_{\mathrm{B}}^{(\tilde{\beta})}+\mathcal{G}_{\mathrm{B}}^{(U)}, \tag{37}$$

where $\mathcal{G}$'s are given in Appendix B. In Eqs. (36) and (37), the first terms are proportional to Δc. The forms of the terms are the same as those in the conserved system[3] except that Δc depends on the impingement rate, and the terms cause the step wandering. The second terms are proportional to the impingement rate. The third terms are proportional to the step stiffness and the forth terms come from the repulsive interaction potential.

$\mathcal{G}_{\mathrm{A,B}}^{(F_{\mathrm{im}})}$ are proportional to the impingement rate and smaller than $\mathcal{G}_{\mathrm{A,B}}^{(D)}$ when the impingement rate is small. The second terms in Eqs. (36) and (37) are negligible and the form of the evolution equation is the same as that without evaporation.[3] Then, the motion of the steps is probably similar to that in the conserved system: grooves are symmetric in the y direction. With increasing the impingement rate, the second terms become more important than the first terms. To see the effect of the impingement on the step wandering, we analyze the step motion only with the second terms. When the step distance is small enough $\Lambda_{\parallel q}l$, $\Lambda_{\perp q}l\ll1$, the linearized evolution equations are given by

$$\frac{d\zeta_{\mathrm{A}}}{dt}=-\frac{\Omega(D_{\perp}^{2}-D_{\parallel}^{2})F_{\mathrm{im}}}{6D_{\perp}D_{\parallel}}\left(\zeta_{A}-\frac{1}{2}\zeta_{B}\right)q^{2}, \tag{38}$$

$$\frac{d\zeta_{\mathrm{B}}}{dt}=\frac{\Omega(D_{\perp}^{2}-D_{\parallel}^{2})F_{\mathrm{im}}}{6D_{\perp}D_{\parallel}}\left(\zeta_{B}-\frac{1}{2}\zeta_{A}\right)q^{2}. \tag{39}$$

The linear amplification rates are

$$\omega_{\pm}=\pm\frac{\sqrt{3}\Omega^{2}(D_{\perp}^{2}-D_{\parallel}^{2})F_{\mathrm{im}}}{12D_{\perp}D_{\parallel}}q^{2}. \tag{40}$$

The relation between amplitudes, ζ_{A} and ζ_{B} for the decaying mode ω_{-} is $\zeta_{\mathrm{A}}=(2+\sqrt{3})\zeta_{\mathrm{B}}$. The relation for the growing mode ω_{+} is $\zeta_{\mathrm{A}}=(2-\sqrt{3})\zeta_{\mathrm{B}}$, and the amplitude of $\mathrm{S_A}$ is smaller than that of $\mathrm{S_B}$. Without impingement, the relation of the two amplitudes is $\zeta_{\mathrm{A}}=\zeta_{\mathrm{B}}$, but the two amplitudes are forced to be different from each other by the impingement. Then, the behaviors of the step wandering, e.g., the wavelength of the wandering, the amplification rate, may change with increasing the impingement rate.

Figure 5 shows snapshots of the late stage of the step wandering. Without the impingement [Fig. 5(a)], the form of wandering step is sinusoidal and symmetric in the y-direction. The valleys and the hills have the same width. With the impingement [Figs. 5(b) and 5(c)], the width of the hills is wider than that of the valleys, and the form is asymmetric in the y direction: the hill is flat and the width of the hills is larger than that of the valleys. When the impingement is present, the coarsening of the width of grooves occurs with

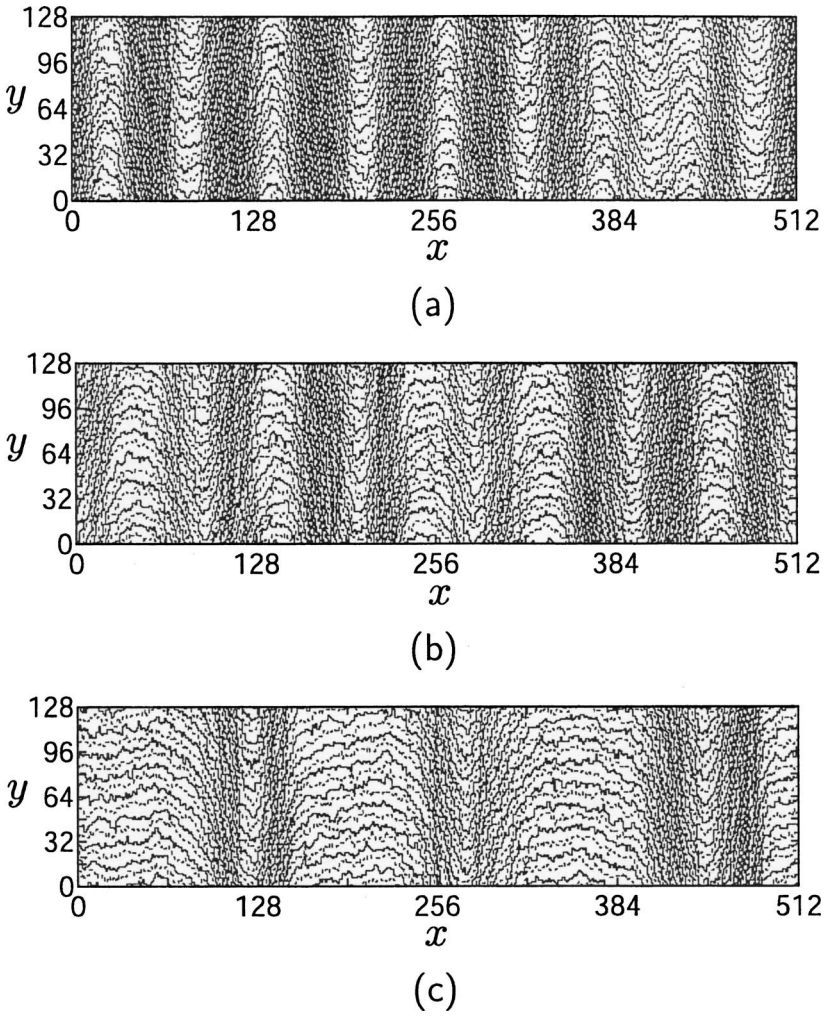

FIG. 5. Snapshots of the step wandering with step-up drift during growth: (a) $F_{\mathrm{im}}=0.0$ at $t=9.9\times10^6$, (b) $F_{\mathrm{im}}=0.003$ at $t=9.5\times10^6$, and (c) $F_{\mathrm{im}}=0.005$ at $t=9.2\times10^6$.

increasing the amplitude of step fluctuation, which is the same as that in the conserved system.

The change of the wandering pattern affects the growth rate of step width. Figure 6 shows the time evolution of step width with various impingement rates. When the impingement rate is small, the growth rate is hardly changed by the impingement. When the impingement rate is large, the growth of step width becomes slow. However, irrespective of the impingement rate, the step width increases as $t^{1/2}$.

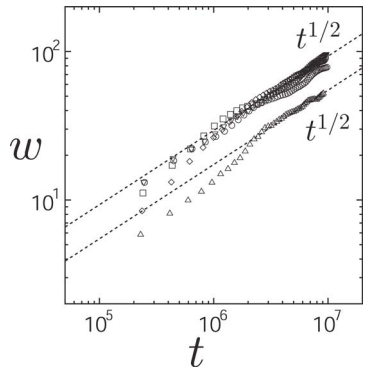

FIG. 6. Time evolution of the step width during growth: ○ without impingement, ▽ with $F_{\mathrm{im}}=0.001$, ◇ with $F_{\mathrm{im}}=0.003$, and △ with $F_{\mathrm{im}}=0.005$.

V. SUMMARY AND DISCUSSION

In this paper, we studied the effect of evaporation and impingement on the drift-induced step wandering with anisotropic surface diffusion. With evaporation, diffusional effect extends only up to two finite surface diffusion lengths. When the surface diffusion lengths are longer than the uniform step distance, the step motion hardly changes from the behavior observed without evaporation. The form of wandering step is sinusoidal and step width increases as $t^{1/2}$. When the evaporation is so strong that at least one of the surface diffusion lengths is comparable or shorter than the step distance, the form of wandering step changes: the narrow hill and the wide valley appear. In this case, the step width saturates ultimately.

If the impingement is present, the form of wandering steps changes with the impingement rate. When the rate is small, the wandering step is sinusoidal as that without evaporation, but with increasing the rate, the hills become wide and flat. Albeit with this form variation, the step width increases as $t^{1/2}$ irrespective of the impingement rate.

On the Si(001) vicinal face, the step wandering was observed in sublimation.[2] On the vicinal face the surface diffusion length is a few μm, which is much longer than the step distance, and the effect of the evaporation is expected to be weak. The fact that the form of grooves observed in the experiment[2] is sinusoidal supports this expectation, and we conclude that the effect the evaporation is negligible in the experiment[2] in spite of the high temperatures (990 °C and 1040 °C). As for the time evolution of the grooves, it is not reported in Ref. 2. If the depth of grooves, which is proportional to the step width, is measured, it will increase with time as $\sim t^{1/2}$.

To observe the impingement effect on the step wandering, a growth experiment is necessary. It has not been carried out so far, but seems feasible on a Si(001) surface as well as on the Si(111) vicinal face.[4] If a similar experiment is carried out on the Si(001) vicinal face, it corresponds to our simulation for the growing vicinal face without evaporation. We expect to observe the surface with narrow grooves and wide hills (Fig. 5), and that the depth of the grooves increases as $t^{1/2}$ (Fig. 6). The absolute amplitude of the growth rate of the depth decreases with increasing the impingement rate, but the exponent does not change. In addition to the asymmetric step pattern, distinct feature of the wandering during growth is that the wavelength increases as the impingement rate (Fig. 5). This is in contrast to other wandering instabilities where the characteristic wavelength decreases as the impingement rate increases.[5,8,17–19] Thus the experiment on a growing Si(001) vicinal face will be a good test to judge if the proposed mechanism for the step instabilities is active.

ACKNOWLEDGMENTS

This work was supported by a Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science. M.U. and Y.S. benefited from the interuniversity cooperative research program of the Institute for Materials Research, Tohoku University.

APPENDIX A: LINEAR EVOLUTION EQUATION WITH EVAPORATION

In Eqs. (19) and (20), the terms $\mathcal{F}_{\mathrm{A}}^{(D)}$ and $\mathcal{F}_{\mathrm{B}}^{(D)}$, which cause the step wandering, are given by

$$\begin{aligned}\mathcal{F}_{\mathrm{A}}^{(D)} = &-\Omega D_{\perp}\left(\Lambda_{\perp q}\frac{\cosh\Lambda_{\perp q}l_{\mathrm{B}}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)\\ &\times\left[\left(\Lambda_{\perp}\frac{\cosh\Lambda_{\perp}l_{\mathrm{B}}}{\sinh\Lambda_{\perp}l_{\mathrm{B}}}-\frac{f}{2}\right)c_{\mathrm{A}}-\frac{\Lambda_{\perp}e^{-fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp}l_{\mathrm{B}}}c_{\mathrm{B}}\right]\zeta_{\mathrm{A}}\\ &-\Omega D_{\perp}\frac{\Lambda_{\perp q}e^{-fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}\left[-\frac{\Lambda_{\perp}e^{fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp}l_{\mathrm{B}}}c_{\mathrm{A}}\right.\\ &\left.+\left(\Lambda_{\perp}\frac{\cosh\Lambda_{\perp}l_{\mathrm{B}}}{\sinh\Lambda_{\perp}l_{\mathrm{B}}}+\frac{f}{2}\right)c_{\mathrm{B}}\right]\zeta_{\mathrm{B}}\\ &-\Omega D_{\parallel}\left(\Lambda_{\parallel q}\frac{\cosh\Lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}-\frac{f}{2}\right)\\ &\times\left[-\left(\Lambda_{\parallel}\frac{\cosh\Lambda_{\parallel}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel}l_{\mathrm{A}}}+\frac{f}{2}\right)c_{\mathrm{A}}+\frac{\Lambda_{\parallel}e^{fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel}l_{\mathrm{A}}}c_{\mathrm{B}}\right]\zeta_{\mathrm{A}}\\ &-\Omega D_{\parallel}\frac{\Lambda_{\parallel q}e^{fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}\left[\frac{\Lambda_{\parallel}e^{-fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel}l_{\mathrm{A}}}c_{\mathrm{A}}\right.\\ &\left.-\left(\Lambda_{\parallel}\frac{\cosh\Lambda_{\parallel}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel}l_{\mathrm{A}}}-\frac{f}{2}\right)c_{\mathrm{B}}\right]\zeta_{\mathrm{B}},\end{aligned}\tag{A1}$$

$$\begin{aligned}\mathcal{F}_{\mathrm{B}}^{(D)} = &-\Omega D_{\parallel}\left(\Lambda_{\parallel q}\frac{\cosh\Lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)\left[\left(\Lambda_{\parallel}\frac{\cosh\Lambda_{\parallel}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel}l_{\mathrm{A}}}-\frac{f}{2}\right)c_{\mathrm{B}}\right.\\ &\left.-\frac{\Lambda_{\parallel}e^{-fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel}l_{\mathrm{A}}}c_{\mathrm{A}}\right]\zeta_{\mathrm{B}}-\Omega D_{\parallel}\frac{\Lambda_{\parallel q}e^{-fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}\left[-\frac{\Lambda_{\parallel}e^{fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel}l_{\mathrm{A}}}c_{\mathrm{B}}\right.\\ &\left.+\left(\Lambda_{\parallel}\frac{\cosh\Lambda_{\parallel}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel}l_{\mathrm{A}}}+\frac{f}{2}\right)c_{\mathrm{A}}\right]\zeta_{\mathrm{A}}-\Omega D_{\perp}\left(\Lambda_{\perp q}\frac{\cosh\Lambda_{\perp q}l_{\mathrm{B}}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}\right.\\ &\left.-\frac{f}{2}\right)\left[-\left(\Lambda_{\perp}\frac{\cosh\Lambda_{\perp}l_{\mathrm{B}}}{\sinh\Lambda_{\perp}l_{\mathrm{B}}}+\frac{f}{2}\right)c_{\mathrm{B}}+\frac{\Lambda_{\perp}e^{fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp}l_{\mathrm{B}}}c_{\mathrm{A}}\right]\zeta_{\mathrm{B}}\\ &-\Omega D_{\perp}\frac{\Lambda_{\perp q}e^{fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}\left[\frac{\Lambda_{\perp}e^{-fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp}l_{\mathrm{B}}}c_{\mathrm{B}}-\left(\Lambda_{\perp}\frac{\cosh\Lambda_{\perp}l_{\mathrm{B}}}{\sinh\Lambda_{\perp}l_{\mathrm{B}}}\right.\right.\\ &\left.\left.-\frac{f}{2}\right)c_{\mathrm{A}}\right]\zeta_{\mathrm{A}},\end{aligned}\tag{A2}$$

where $\Lambda_{\perp q}$ and $\Lambda_{\parallel q}$ are defined as

$$\Lambda_{\perp q}=\frac{1}{2}\sqrt{f^2+4\left(\frac{1}{x_{\perp}^2}+\frac{D_{\parallel}}{D_{\perp}}q^2\right)},\tag{A3}$$

$$\Lambda_{\parallel q}=\frac{1}{2}\sqrt{f^2+4\left(\frac{1}{x_{\parallel}^2}+\frac{D_{\perp}}{D_{\parallel}}q^2\right)}.\tag{A4}$$

The terms $\mathcal{F}_{\mathrm{A}}^{(\tilde{\beta})}$ and $\mathcal{F}_{\mathrm{B}}^{(\tilde{\beta})}$, which originate from the step stiffness and suppress the step wandering, are given by

$$\begin{aligned}\mathcal{F}_{\mathrm{A}}^{(\tilde{\beta})} = &-D_{\perp}\frac{\Omega^2\tilde{\beta}}{k_{\mathrm{B}}T}q^2\left[\left(\Lambda_{\perp q}\frac{\cosh\Lambda_{\perp q}l_{\mathrm{B}}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)\zeta_{\mathrm{A}}\right.\\ &\left.-\frac{\Lambda_{\perp q}e^{-fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}\zeta_{\mathrm{B}}\right]-D_{\parallel}\frac{\Omega^2\tilde{\beta}}{k_{\mathrm{B}}T}q^2\left[\left(\Lambda_{\parallel q}\frac{\cosh\Lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}\right.\right.\\ &\left.\left.-\frac{f}{2}\right)\zeta_{\mathrm{A}}-\frac{\Lambda_{\parallel q}e^{fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}\zeta_{\mathrm{B}}\right],\end{aligned}\tag{A5}$$

$$\begin{aligned}\mathcal{F}_{\mathrm{B}}^{(\tilde{\beta})} = &-D_{\parallel}\frac{\Omega^2\tilde{\beta}}{k_{\mathrm{B}}T}q^2\left[\left(\Lambda_{\parallel q}\frac{\zeta_{\mathrm{B}}\cosh\Lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)\zeta_{\mathrm{B}}\right.\\ &\left.-\frac{\Lambda_{\parallel q}e^{-fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}\zeta_{\mathrm{A}}\right]-D_{\perp}\frac{\Omega^2\tilde{\beta}}{k_{\mathrm{B}}T}q^2\left[\left(\Lambda_{\perp q}\frac{\cosh\Lambda_{\perp q}l_{\mathrm{B}}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}\right.\right.\\ &\left.\left.-\frac{f}{2}\right)\zeta_{\mathrm{B}}-\frac{\Lambda_{\perp q}e^{fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}\zeta_{\mathrm{A}}\right].\end{aligned}\tag{A6}$$

The terms $\mathcal{F}_{\mathrm{A}}^{(U)}$ and $\mathcal{F}_{\mathrm{B}}^{(U)}$, which originate from the step-step repulsion, are given by

$$\mathcal{F}_{\mathrm{A}}^{(U)} = -\Omega D_{\perp g}\left[\left(\Lambda_{\perp q}\frac{\cosh\Lambda_{\perp q}l_{\mathrm{B}}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)+\frac{\Lambda_{\perp q}e^{-fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}\right]\times(\zeta_{\mathrm{A}}-\zeta_{\mathrm{B}}) - \Omega D_{\parallel g}\left[\left(\Lambda_{\parallel q}\frac{\cosh\Lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}-\frac{f}{2}\right)+\frac{\Lambda_{\parallel q}e^{fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}\right](\zeta_{\mathrm{A}}-\zeta_{\mathrm{B}}), \tag{A7}$$

$$\mathcal{F}_{\mathrm{B}}^{(U)} = -\Omega D_{\parallel g}\left[\left(\Lambda_{\parallel q}\frac{\cosh\Lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)-\frac{\Lambda_{\parallel q}e^{-fl_{\mathrm{A}}/2}}{\sinh\Lambda_{\parallel q}l_{\mathrm{A}}}\right](\zeta_{\mathrm{B}}-\zeta_{\mathrm{A}}) - \Omega D_{\perp g}\left[\left(\Lambda_{\perp q}\frac{\cosh\Lambda_{\perp q}l_{\mathrm{B}}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}-\frac{f}{2}\right)-\frac{\Lambda_{\perp q}e^{fl_{\mathrm{B}}/2}}{\sinh\Lambda_{\perp q}l_{\mathrm{B}}}\right]\times(\zeta_{\mathrm{B}}-\zeta_{\mathrm{A}}). \tag{A8}$$

APPENDIX B: LINEAR EVOLUTION EQUATION WITH IMPINGEMENT

In Eqs. (36) and (37), the first terms, $\mathcal{G}_{\mathrm{A}}^{(D)}$ and $\mathcal{G}_{\mathrm{B}}^{(D)}$ are given by

$$\mathcal{G}_{\mathrm{A}}^{(D)} = \frac{\Omega D_{\perp} f\Delta c}{e^{fl_{\mathrm{B}}}-1}\left[\left(\lambda_{\perp q}\frac{\cosh\lambda_{\perp q}l_{\mathrm{B}}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)\zeta_{\mathrm{A}}-\frac{\lambda_{\perp q}e^{\lambda_{\perp q}fl_{\mathrm{B}}/2}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}\zeta_{\mathrm{B}}\right] + \frac{\Omega D_{\parallel} f\Delta c}{1-e^{-fl_{\mathrm{B}}}}\left[\left(-\lambda_{\parallel q}\frac{\cosh\lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)\zeta_{\mathrm{A}}-\frac{\lambda_{\parallel q}e^{-fl_{\mathrm{A}}/2}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}\zeta_{\mathrm{B}}\right], \tag{B1}$$

$$\mathcal{G}_{\mathrm{B}}^{(D)} = \frac{\Omega D_{\parallel} f\Delta c}{1-e^{fl_{\mathrm{A}}}}\left[\left(\lambda_{\parallel q}\frac{\cosh\lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)\zeta_{\mathrm{B}}-\frac{e^{\lambda_{\parallel q}fl_{\mathrm{A}}/2}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}\zeta_{\mathrm{A}}\right] + \frac{\Omega D_{\perp} f\Delta c}{e^{-fl_{\mathrm{B}}}-1}\left[\left(-\lambda_{\perp q}\frac{\cosh\lambda_{\perp q}l_{\mathrm{B}}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)\zeta_{\mathrm{B}} - \frac{\lambda_{\perp q}e^{-fl_{\mathrm{B}}/2}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}\zeta_{\mathrm{A}}\right], \tag{B2}$$

where $\lambda_{\perp q}$ and $\lambda_{\parallel q}$ are defined as

$$\lambda_{\perp q} = \frac{1}{2}\sqrt{f^2+\frac{4D_{\parallel}}{D_{\perp}}q^2}, \tag{B3}$$

$$\lambda_{\parallel q} = \frac{1}{2}\sqrt{f^2+\frac{4D_{\perp}}{D_{\parallel}}q^2}. \tag{B4}$$

The second terms, $\mathcal{G}_{\mathrm{A}}^{(F_{\mathrm{im}})}$ and $\mathcal{G}_{\mathrm{B}}^{(F_{\mathrm{im}})}$ are given by

$$\mathcal{G}_{\mathrm{A}}^{(F_{\mathrm{im}})} = \frac{\Omega^2 F_{\mathrm{im}}}{f}\left[\left(\lambda_{\perp q}\frac{\cosh\lambda_{\perp q}l_{\mathrm{B}}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)\left(1-\frac{fl_{\mathrm{B}}}{e^{fl_{\mathrm{B}}}-1}\right)\zeta_{\mathrm{A}} - \frac{\lambda_{\perp q}e^{-fl_{\mathrm{B}}/2}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}\left(1-\frac{fl_{\mathrm{B}}e^{fl_{\mathrm{B}}}}{e^{fl_{\mathrm{B}}}-1}\right)\zeta_{\mathrm{B}}\right] - \frac{\Omega^2 F_{\mathrm{im}}}{f}\left[\left(\lambda_{\parallel q}\frac{\cosh\lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)\left(1-\frac{fl_{\mathrm{A}}e^{fl_{\mathrm{A}}}}{e^{fl_{\mathrm{A}}}-1}\right)\zeta_{\mathrm{A}} - \frac{\lambda_{\parallel q}e^{fl_{\mathrm{A}}/2}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}\left(1-\frac{fl_{\mathrm{A}}}{e^{fl_{\mathrm{A}}}-1}\right)\zeta_{\mathrm{B}}\right], \tag{B5}$$

$$\mathcal{G}_{\mathrm{B}}^{(\mathrm{im})} = \frac{\Omega^2 F_{\mathrm{im}}}{f}\left[\left(\lambda_{\parallel q}\frac{\cosh\lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)\left(1-\frac{fl_{\mathrm{A}}}{e^{fl_{\mathrm{A}}}-1}\right)\zeta_{\mathrm{B}} - \frac{\lambda_{\parallel q}e^{-fl_{\mathrm{A}}/2}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}\left(1-\frac{fl_{\mathrm{A}}e^{fl_{\mathrm{A}}}}{e^{fl_{\mathrm{A}}}-1}\right)\zeta_{\mathrm{A}}\right] - \frac{\Omega^2 F_{\mathrm{im}}}{f}\left[\left(\lambda_{\perp q}\frac{\cosh\lambda_{\perp q}l_{\mathrm{B}}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)\left(1-\frac{fl_{\mathrm{B}}e^{fl_{\mathrm{B}}}}{e^{fl_{\mathrm{B}}}-1}\right)\zeta_{\mathrm{B}} - \frac{\lambda_{\perp q}e^{-fl_{\mathrm{B}}/2}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}\left(1-\frac{fl_{\mathrm{B}}}{e^{fl_{\mathrm{B}}}-1}\right)\zeta_{\mathrm{A}}\right]. \tag{B6}$$

The terms $\mathcal{G}_{\mathrm{A}}^{(\tilde{\beta})}$ and $\mathcal{G}_{\mathrm{B}}^{(\tilde{\beta})}$, which are derived from the step stiffness and suppress the step wandering, are given by

$$\mathcal{G}_{\mathrm{A}}^{(\tilde{\beta})} = -D_{\perp}\frac{\Omega^2\tilde{\beta}}{k_{\mathrm{B}}T}q^2\left[\left(\lambda_{\perp q}\frac{\cosh\lambda_{\perp q}l_{\mathrm{B}}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)\zeta_{\mathrm{A}} - \frac{\lambda_{\perp q}e^{-fl_{\mathrm{B}}/2}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}\zeta_{\mathrm{B}}\right] - D_{\parallel}\frac{\Omega^2\tilde{\beta}}{k_{\mathrm{B}}T}q^2\left[\left(\lambda_{\parallel q}\frac{\cosh\lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}-\frac{f}{2}\right)\zeta_{\mathrm{A}} - \frac{\lambda_{\parallel q}e^{fl_{\mathrm{A}}/2}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}\zeta_{\mathrm{B}}\right], \tag{B7}$$

$$\mathcal{G}_{\mathrm{B}}^{(\tilde{\beta})} = -D_{\parallel}\frac{\Omega^2\tilde{\beta}}{k_{\mathrm{B}}T}q^2\left[\left(\lambda_{\parallel q}\frac{\zeta_{\mathrm{B}}\cosh\lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)\zeta_{\mathrm{B}} - \frac{\lambda_{\parallel q}e^{-fl_{\mathrm{A}}/2}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}\zeta_{\mathrm{A}}\right] - D_{\perp}\frac{\Omega^2\tilde{\beta}}{k_{\mathrm{B}}T}q^2\left[\left(\lambda_{\perp q}\frac{\cosh\lambda_{\perp q}l_{\mathrm{B}}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}} - \frac{f}{2}\right)\zeta_{\mathrm{B}} - \frac{\lambda_{\perp q}e^{fl_{\mathrm{B}}/2}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}\zeta_{\mathrm{A}}\right]. \tag{B8}$$

The terms $\mathcal{G}_{\mathrm{A}}^{(U)}$ and $\mathcal{G}_{\mathrm{A}}^{(U)}$, which are derived from the step-step repulsive interaction potential, are given by

$$\mathcal{G}_{\mathrm{A}}^{(U)} = -\Omega D_{\perp g}\left[\left(\lambda_{\perp q}\frac{\cosh\lambda_{\perp q}l_{\mathrm{B}}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}+\frac{f}{2}\right)-\frac{\lambda_{\perp q}e^{-fl_{\mathrm{B}}/2}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}\right](\zeta_{\mathrm{A}}-\zeta_{\mathrm{B}}) - \Omega D_{\parallel g}\left[\left(\lambda_{\parallel q}\frac{\cosh\lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}-\frac{f}{2}\right)-\frac{\lambda_{\parallel q}e^{fl_{\mathrm{A}}/2}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}\zeta_{\mathrm{B}}\right]\times(\zeta_{\mathrm{A}}-\zeta_{\mathrm{B}}), \tag{B9}$$

$$\mathcal{G}_{\mathrm{B}}^{(U)} = -\Omega D_{\parallel g}\left[\left(\lambda_{\parallel q}\frac{\zeta_{\mathrm{B}}\cosh\lambda_{\parallel q}l_{\mathrm{A}}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}+\frac{f}{2}\right)-\frac{\lambda_{\parallel q}e^{-fl_{\mathrm{A}}/2}}{\sinh\lambda_{\parallel q}l_{\mathrm{A}}}\right](\zeta_{\mathrm{B}}-\zeta_{\mathrm{A}}) - \Omega D_{\perp g}\left[\left(\lambda_{\perp q}\frac{\cosh\lambda_{\perp q}l_{\mathrm{B}}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}-\frac{f}{2}\right)-\frac{\lambda_{\perp q}e^{fl_{\mathrm{B}}/2}}{\sinh\lambda_{\perp q}l_{\mathrm{B}}}\right]\times(\zeta_{\mathrm{B}}-\zeta_{\mathrm{A}}). \tag{B10}$$

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