Repulsion-mediated step wandering on a Si(001) vicinal face

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Repulsion-mediated step wandering on a Si(001) vicinal face

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With a Si(001) vicinal surface in mind, we study step wandering instability on a vicinal surface with an anisotropic surface diffusion whose orientation dependence alternates on each consecutive terrace. In a conserved system step wandering takes place with step-up adatom drift. Repulsive interaction between steps is found indispensable for the instability. Monte Carlo simulation with a strong repulsive step interaction confirms the result of linear stability analysis, and further shows that in-phase step wandering produces straight grooves. Grooves widen as their amplitudes increase in proportion to the square root of time.

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I. INTRODUCTION

On a vicinal surface of a crystal, steps undergo two types of dynamical instabilities: wandering and bunching. Step wandering is the instability for step deformation along the step, and step bunching is the one for the interstep distance.[1] Both instabilities are caused by some asymmetry in the surface diffusion field. There are many effects which cause the asymmetry, and the drift flow of adsorbed atoms (adatoms) is one of them. On Si(111) and Si(001) vicinal faces, a direct electric current induces drift of adatoms and the instabilities have been observed under its application.[2]

The Si(001) surface is reconstructed and forms rows of dimerized atoms arranged in a 2×1 unit cell (Fig. 1). On the reconstructed surface, the adatom surface diffusion is anisotropic such that it takes place more easily perpendicular to the dimers (parallel to the dimer rows) than in parallel. On a vicinal face terraces of different heights are bounded by steps. On consecutive terraces the dimer orientation alternates, and we call the 1×2 terrace $\mathrm{T_A}$ and the 2×1 terrace $\mathrm{T_B}$.

Due to the alternation of the orientation of fast surface diffusion on different terraces, conditions of the step instabilities for a Si(001) vicinal face differ from those for a Si(111) vicinal face. Experimentally, bunching is observed on a (001) vicinal face with a finite current irrespective of its direction[3–5] and the step wandering with the step-up current.[6] Since the drift is believed to be parallel to the current,[7,8] the drift direction that will cause the step wandering is opposite to that on a Si(111) vicinal face.

Theoretically, step bunching on a Si(001) vicinal face has been studied by one-dimensional step flow models[9–11] and by Monte Carlo simulations.[12] When the alternation of anisotropic surface diffusion is taken into account, the step bunching instability is found irrespective of the drift direction, in agreement with the experiments.[3–5] On the contrary, to our best knowledge, there is no theoretical study on the step wandering on a Si(001) vicinal face so far, which we undertake in this paper.

We find that strong step repulsion prevents steps from colliding and maintains an alternating terrace structure. On these terraces, due to the step repulsion, a diffusion current perpendicular to the average step direction arises if steps are tilted, and it causes a wandering instability. This step wandering is unique, since it happens only on a vicinal face, and therefore is truly a many-body effect.

A simple model for a Si(001) vicinal face with a drift of adatoms is introduced in Sec. II. We show, by a linear stability analysis in Sec. III, that the steady state with step-up drift is unstable and wandering instability occurs. A heuristic analysis in Sec. IV shows that the wandering instability is similar to that found in other conserved systems.[13,14] In Sec. V, with Monte Carlo simulations, we confirm the above theoretical predictions and also study the growth law of the wandering amplitude. In Sec. VI we give a brief discussion on the character of the present instability and interpret recent experiments[6] on Si(001).

II. MODEL

Atoms detached from steps migrate on terraces and attach to some steps. For wandering instability, adatom drift is necessary in addition to diffusive motion. Evaporation and impingement are omitted. Steps run parallel to the x direction on average, and the positive y direction is chosen in the step-down direction. The drift is assumed in the y direction. With the anisotropy of the diffusion coefficient, the diffusion equation of adatom density $c(x,y,t)$ is expressed as

$$\frac{\partial c}{\partial t}=D_x\frac{\partial^2 c}{\partial x^2}+D_y\frac{\partial^2 c}{\partial y^2}-fD_y\frac{\partial c}{\partial y}, \tag{1}$$

where D_x is the diffusion coefficient in the x direction, D_y is in the y direction, and f $(=F/k_\mathrm{B}T)$ is the force to induce the drift divided by the temperature. The meaning of D_x and D_y depends on which terrace we are discussing, $\mathrm{T_A}$ or $\mathrm{T_B}$, and we come to this point later. For simplicity, we assume that the step kinetics is fast enough that the adatom density attains its local equilibrium value at each step:

$$c|_\pm=c_\mathrm{eq}^0\left(1+\frac{\Omega\tilde{\beta}}{k_\mathrm{B}T}\kappa+\frac{\Omega}{k_\mathrm{B}T}\frac{\partial U}{\partial y}\right). \tag{2}$$

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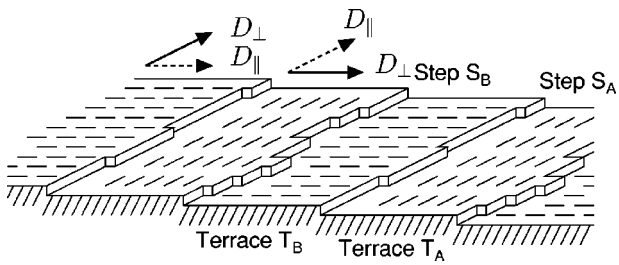

FIG. 1. A Si(001) vicinal face. Short lines on terraces represent dimers.

Here $+(-)$ indicates the lower (upper) side of the step, c_{eq}^0 is the equilibrium adatom density of a free straight step, Ω the atomic area, $\tilde{\beta}$ the step stiffness, κ the curvature of the step, and U the step-step interaction potential. We assume that U is a function of the step distance l in the y direction as[15] $U=A(l_+^{-2}+l_-^{-2})$ with a positive constant A, corresponding to step repulsion. There is a more detailed model where U is expressed by an integration of the force dipole along the step.[16] But in the linear analysis the complication is shown to be incorporated into the renormalization of the stiffness. Therefore, we use the simple form for U here.

By solving Eq. (1) with the boundary conditions in the quasistatic approximation ($\partial c/\partial t=0$), the adatom density c and then the adatom current $\boldsymbol{j}$ are determined. The step velocity is given by

$$V=\Omega\hat{\boldsymbol{n}}\cdot(\boldsymbol{j}|_- - \boldsymbol{j}|_+), \tag{3}$$

where $\hat{\boldsymbol{n}}$ is the normal vector in the step-down direction.

Due to the different orientation of the dimer rows on T_A and T_B, a set of diffusion coefficients (D_x,D_y) corresponds to different combinations: $(D_x,D_y)=(D_\parallel,D_\perp)$ on T_A and $(D_x,D_y)=(D_\perp,D_\parallel)$ on T_B, and $D_\perp$ is larger than $D_\parallel$. Since the step S_B is rougher than S_A on a Si(001) vicinal face, step parameters are different in general for the two types of steps, S_A and S_B, but for simplicity, we neglect these differences.

III. STABILITY ANALYSIS

On a flat vicinal face where parallel steps are arranged equidistantly, the adatom concentration is homogeneous as c_{eq}^0. The step velocities V_A and V_B of the steps S_A and S_B are calculated as

$$V_A=-V_B=-\frac{\Omega F(D_\perp-D_\parallel)c_{eq}^0}{k_BT}. \tag{4}$$

Since the step velocities V_A and V_B are nonvanishing and opposite for a finite drift ($F\neq 0$), the flat vicinal face is unstable against step pairing. Without the repulsive step-step interaction, the adatom concentration is as homogeneous as c_{eq}^0, irrespective of the step distance. The steps move with the velocities V_A and V_B given above, and by coalescence the surface is covered by one type of terrace, for instance, T_A for positive F since $D_\perp>D_\parallel$.

If the repulsive interaction is granted, the difference of terrace widths l_A and l_B of terraces T_A and T_B causes the difference of the equilibrium adatom densities c_A and c_B at steps S_A and S_B. Then the steady state with vanishing step velocities can be established even with the drift to be

$$\frac{D_\perp(c_Ae^{fl_A}-c_B)}{e^{fl_A}-1}=\frac{D_\parallel(c_Be^{fl_B}-c_A)}{e^{fl_B}-1}. \tag{5}$$

Since the average terrace width of the vicinal face is fixed to l, wide and narrow terraces appear alternately as $l_A=l+\delta l/2$ and $l_B=l-\delta l/2$, and the equilibrium densities also alternate as $c_A=c_{eq}^0-\Delta c/2$ and $c_B=c_{eq}^0+\Delta c/2$, respectively. For a small drift fl and the strong repulsive interaction, Eq. (5) gives the density difference $\Delta c=c_B-c_A$ as

$$\Delta c=\frac{2(D_\parallel-D_\perp)c_{eq}^0\tanh(fl_A/2)\tanh(fl_B/2)}{D_\parallel\tanh(fl_B/2)+D_\perp\tanh(fl_A/2)}\approx\frac{D_\perp-D_\parallel}{D_\perp+D_\parallel}c_{eq}^0fl. \tag{6}$$

On the other hand, from the step-step repulsion, Δc is given by

$$\Delta c\approx\Delta g\,\delta l, \tag{7}$$

where δl is the difference of the terrace width and Δg is

$$\Delta g=\frac{12A\Omega c_{eq}^0}{k_BTl^4}. \tag{8}$$

From Eqs. (6) and (7), the terrace width difference δl is given by

$$\frac{\delta l}{l}=\frac{Fl^4(D_\perp-D_\parallel)}{12\Omega A(D_\perp+D_\parallel)}. \tag{9}$$

Without repulsive interaction $A=0$, the terrace width cannot remain finite. Also the above equation indicates that the deviation of the terrace width $\delta l/l$ is small under a very strong step repulsion.

We now study the stability of this steady state with alternating terrace widths under the adatom drift. The evolution of the perturbation $\zeta_A(t)e^{iqx}$ to S_A and $\zeta_B(t)e^{iqx}$ to S_B are governed by

$$\begin{aligned}\frac{d\zeta_A}{dt}=&\frac{\Omega D_\perp f\Delta c}{(e^{fl_A}-1)}\left[\frac{f}{2}\zeta_A+\frac{\alpha_A(\zeta_A\cosh\alpha_Al_A-\zeta_Be^{fl_A/2})}{\sinh\alpha_Al_A}\right]\\&+\frac{\Omega D_\parallel f\Delta c}{(1-e^{-fl_B})}\left[\frac{f}{2}\zeta_A-\frac{\alpha_B(\zeta_A\cosh\alpha_Bl_B-\zeta_Be^{-fl_B/2})}{\sinh\alpha_Bl_B}\right]\\&-\Omega D_\perp\Gamma q^2\left[\frac{f}{2}\zeta_A+\frac{\alpha_A(\zeta_A\cosh\alpha_Al_A-\zeta_Be^{-fl_A/2})}{\sinh\alpha_Al_A}\right]\\&+\Omega D_\parallel\Gamma q^2\left[\frac{f}{2}\zeta_A-\frac{\alpha_B(\zeta_A\cosh\alpha_Bl_B-\zeta_Be^{fl_B/2})}{\sinh\alpha_Bl_B}\right]\\&-\Omega D_\perp\Delta g(\zeta_A-\zeta_B)\left[\frac{f}{2}+\frac{\alpha_A(\cosh\alpha_Al_A+e^{-fl_A/2})}{\sinh\alpha_Al_A}\right]\end{aligned}$$

$$+\Omega D_{\parallel}\Delta g(\zeta_A-\zeta_B)\left[\frac{f}{2}-\frac{\alpha_B(\cosh\alpha_B l_B+e^{fl_B/2})}{\sinh\alpha_B l_B}\right], \tag{10}$$

$$\begin{aligned}\frac{d\zeta_B}{dt}=&\frac{\Omega D_{\parallel}f\Delta c}{(1-e^{fl_B})}\left[\frac{f}{2}\zeta_B+\frac{\alpha_B(\zeta_B\cosh\alpha_B l_B-\zeta_A e^{fl_B/2})}{\sinh\alpha_B l_B}\right]\\&+\frac{\Omega D_{\perp}f\Delta c}{(e^{-fl_A}-1)}\left[\frac{f}{2}\zeta_B-\frac{\alpha_A(\zeta_B\cosh\alpha_A l_A-\zeta_A e^{-fl_A/2})}{\sinh\alpha_A l_A}\right]\\&-\Omega D_{\parallel}\Gamma q^2\left[\frac{f}{2}\zeta_B+\frac{\alpha_B(\zeta_B\cosh\alpha_B l_B-\zeta_A e^{-fl_B/2})}{\sinh\alpha_B l_B}\right]\\&+\Omega D_{\perp}\Gamma q^2\left[\frac{f}{2}\zeta_B-\frac{\alpha_A(\zeta_B\cosh\alpha_A l_A-\zeta_A e^{fl_A/2})}{\sinh\alpha_A l_A}\right]\\&-\Omega D_{\parallel}\Delta g(\zeta_B-\zeta_A)\left[\frac{f}{2}+\frac{\alpha_B(\cosh\alpha_B l_B+e^{-fl_B/2})}{\sinh\alpha_B l_B}\right]\\&+\Omega D_{\perp}\Delta g(\zeta_B-\zeta_A)\left[\frac{f}{2}-\frac{\alpha_A(\cosh\alpha_A l_A+e^{fl_A/2})}{\sinh\alpha_A l_A}\right],\end{aligned} \tag{11}$$

where $\Gamma=\Omega c_{eq}^0\tilde{\beta}/k_BT$, and

$$\alpha_A=\sqrt{\frac{f^2}{4}+\frac{D_{\parallel}}{D_{\perp}}q^2}, \tag{12}$$

$$\alpha_B=\sqrt{\frac{f^2}{4}+\frac{D_{\perp}}{D_{\parallel}}q^2}. \tag{13}$$

When the step distance is as small as $\alpha l\ll 1$, Eqs. (10) and (11) are approximated as

$$\begin{aligned}\frac{d\zeta_A}{dt}=-\frac{d\zeta_B}{dt}=&\frac{\Omega\Delta c}{l^2}(D_{\perp}-D_{\parallel})(\zeta_A-\zeta_B)-\frac{\Omega}{l}(D_{\perp}+D_{\parallel})\\&\times(\Gamma q^2+2\Delta g)(\zeta_A-\zeta_B),\end{aligned} \tag{14}$$

where we neglect the difference of the step distance. When the fluctuations $\zeta_A(x,t)$ and $\zeta_B(x,t)$ increase proportionally to $e^{\omega t}$, the amplification rate ω is given by

$$\omega_1=2\frac{\Omega\Delta c}{l^2}(D_{\perp}-D_{\parallel})-2\frac{\Omega}{l}(D_{\perp}+D_{\parallel})(\Gamma q^2+2\Delta g), \tag{15}$$

$$\omega_2=0. \tag{16}$$

$\omega=\omega_1$ is the rate of amplification for the out-of-phase fluctuation; $\zeta_A=-\zeta_B$. Since we are considering the limit of strong step repulsion (or weak drift), Δg is quite large to suppress the out-of-phase fluctuation and ω_1 is negative. $\omega=\omega_2$ is the amplification rate for the in-phase fluctuation; $\zeta_A=\zeta_B$. $\omega_2=0$ means the step is marginal to the in-phase step wandering, since the step repulsion is ineffective for the deformation which does not alter the step separation. However, by assuming $\zeta_A=\zeta_B$, Eqs. (10) and (11) can be easily expanded one-order higher in the terrace widths l.

For the fluctuations $\zeta_A(x,t)=\zeta_B(x,t)=\zeta_q e^{iqx}e^{\omega_q t}$, the amplification rate for small q is given by

$$\omega_q=\alpha_2 q^2-\alpha_4 q^4, \tag{17}$$

where the coefficients α_2 and α_4 are

$$\alpha_2=-\frac{\Omega(D_{\perp}-D_{\parallel})\Delta c}{2}, \tag{18}$$

$$\alpha_4=\frac{\Omega^2(D_{\parallel}+D_{\perp})c_{eq}^0\tilde{\beta}l}{2k_BT}. \tag{19}$$

Here we have assumed that the terrace widths are as small as $ql\ll 1$. When the drift is in the step-down direction ($F>0$), the quadratic term in q is negative and the steady state is stable. When the drift is in the step-up direction ($F<0$), the quadratic term is positive. Then the steady state with straight steps is unstable and in-phase step wandering occurs. Thus the first term indicates an instability of the steady state by changing its sign with the drift direction. Note that the wandering is caused by the difference Δc of equilibrium concentrations at the steps originated from the step repulsion. Thus the step repulsion is indispensable for the establishment of wandering instability on a Si(001) vicinal. Also note that there is no critical value for the step-up drift. If the drift changes from step down to step up, steps immediately show the wandering instability, because the Gibbs-Thomson effect gives only a quartic term, higher than the destabilizing quadratic term.

The wavelength of the most unstable mode is given by

$$\lambda_{max}=2\pi\sqrt{\frac{2\alpha_4}{\alpha_2}}=2\pi\frac{D_{\perp}+D_{\parallel}}{D_{\perp}-D_{\parallel}}\sqrt{\frac{2\Omega\tilde{\beta}}{|F|}}. \tag{20}$$

The characteristic wavelength is inversely proportional to the square root of the external field E which causes the drift: $\lambda_{max}\propto 1/\sqrt{E}$.

IV. NONLINEAR ANALYSIS

After the instability sets in, the step deformation amplifies, and a nonlinear analysis is called for. Assuming an in-phase motion of steps due to the strong step repulsion $\zeta_A=\zeta_B=\zeta(x,t)$, a heuristic argument is possible on the nonlinear evolution of the step wandering. This simultaneously reveals the physical origin of the wandering.

We first assume that every step is tilted uniformly from the y direction with an angle θ as

$$\frac{\partial\zeta}{\partial x}=\tan\theta. \tag{21}$$

The adatom density on a terrace T_A ($x\tan\theta<y<l_A+x\tan\theta$) is given by

$$c(x,y)=(c_A-c_B)\frac{e^{\tilde{f}_A(y-\tan\theta x)}-e^{\tilde{f}_A l_A}}{1-e^{\tilde{f}_A l_A}}+c_B, \tag{22}$$

where $\tilde{f}_A$ is defined as

$$\tilde{f}_A = \frac{fD_\perp}{D_\perp + D_\parallel \tan^2\theta}. \tag{23}$$

Here c_A and c_B are the adatom concentrations on terraces A and B, respectively, in the steady state. They differ from the values determined by Eq. (5) since the steps are uniformly tilted.

Then adatom current j_x^A in the x direction and j_y^A in the y direction are given by

$$j_x^A = -D_\parallel \frac{\partial c}{\partial x} = D_\parallel (c_A - c_B) \frac{e^{\tilde{f}_A (y - \tan\theta x)} \tilde{f}_A \tan\theta}{1 - e^{\tilde{f}_A l_A}}, \tag{24}$$

$$j_y^A = -D_\perp \frac{\partial c}{\partial y} + D_\perp f c = \frac{D_\perp e^{\tilde{f}_A (y - \tan\theta x)}}{1 - e^{\tilde{f}_A l_A}} (c_A - c_B)(f - \tilde{f}_A) + D_\perp f \frac{c_B - e^{\tilde{f}_A l_A} c_A}{1 - e^{\tilde{f}_A l_A}}. \tag{25}$$

From the above current components, the adatom current perpendicular to the step on a terrace T_A is given by

$$j_\perp^A = -j_x^A \sin\theta + j_y^A \cos\theta = D_\perp f \cos\theta \frac{c_A e^{\tilde{f}_A l_A} - c_B}{e^{\tilde{f}_A l_A} - 1}. \tag{26}$$

Similarly, on a terrace T_B, the corresponding current is given by

$$j_\perp^B = D_\parallel f \cos\theta \frac{c_B e^{\tilde{f}_B l_B} - c_A}{e^{\tilde{f}_B l_B} - 1}, \tag{27}$$

where

$$\tilde{f}_B = \frac{fD_\parallel}{D_\parallel + D_\perp \tan^2\theta}. \tag{28}$$

The steady state is determined by the condition $j_\perp^A = j_\perp^B$. For strong repulsion with $l_A = l_B$, the difference of the equilibrium adatom density depends on the step slope as

$$\Delta c = \frac{D_\perp - D_\parallel}{D_\perp + D_\parallel} f l \cos^2\theta c_{eq}^0, \tag{29}$$

where we use $\tilde{f} l \ll 1$. By comparison with Eq. (6), the step tilting is found to make the amplitude of the concentration difference $|\Delta c|$ smaller by a factor of $\cos^2\theta$ than the case without tilting.

When the tilting angle θ varies from place to place, the nonuniformity causes the step instability, as described in the previous section. Since all steps move in phase and the number of atoms is conserved, the in-phase step motion is controlled by the adatom current in the x direction. The drift current has no x component so that only the diffusion current determines the evolution of step fluctuation.

There are two contributions in the diffusion current. One is the current across the terrace induced by the difference of the equilibrium densities at both ends of the terrace. From Eq. (24), the x component of the total flux on T_A is given by

$$J_x^A = \int_0^{l_A} j_x^A(0,y)\,dy = -D_\parallel (c_A - c_B) \tan\theta. \tag{30}$$

Similarly the x component of the flux on T_B is given by

$$J_x^B = -D_\perp \Delta c \tan\theta. \tag{31}$$

Then, the average flux per step is

$$J_x^{(1)} = \frac{(J_x^A + J_x^B)}{2} \approx -(D_\perp - D_\parallel) \frac{\Delta c}{2} \frac{\partial \zeta}{\partial x}. \tag{32}$$

When $\Delta c < 0$ (i.e., $F < 0$), the flux is an increasing function of the slope and an instability is expected.

The other diffusion current is along the steps due to the chemical-potential change with curvature. Considering that the normal distance between steps for a tilted part is $l_{A,B} \cos\theta$, the flux (per step) passing through the two terraces induced by the chemical-potential gradient is

$$J_x^{(2)} = -\frac{(l_A \cos\theta D_\parallel + l_B \cos\theta D_\perp) c_{eq}^0 \cos\theta}{2 k_B T} \frac{\partial \mu}{\partial x}. \tag{33}$$

The chemical potential μ is determined solely by the Gibbs-Thomson effect $\Omega \tilde{\beta} \kappa$ and is independent of the step repulsion in the present choice of interaction U since the terrace width in the y direction is constant for the in-phase modulation. A more general expression given by Paulin and co-workers[16] might modify the following result quantitatively but not qualitatively.

With the two contributions together, mass conservation leads to the following nonlinear time evolution of the in-phase step deformation $\zeta(x,t)$:

$$\frac{\partial \zeta}{\partial t} = -\frac{\partial [J_x^{(1)} + J_x^{(2)}]}{\partial x} = -\frac{\partial}{\partial x} \left\{ \frac{1}{1+\zeta_x^2} \left[\alpha_2 \zeta_x + \alpha_4 \frac{\partial}{\partial x} \frac{\zeta_{xx}}{(1+\zeta_x^2)^{3/2}} \right] \right\}, \tag{34}$$

where $\zeta_x = \partial\zeta/\partial x$ and $\zeta_{xx} = \partial^2\zeta/\partial x^2$. The coefficients α_2 and α_4 are those in Eq. (17). With $\zeta = \zeta_q e^{iqx + \omega_q t}$ the linear amplification rate ω_q is recovered from Eq. (34). Interestingly, Eq. (34) is the same as the nonlinear equation obtained for other conserved systems,[13,14,16–18] although the mechanism looks very different.

V. MONTE CARLO SIMULATION

To study the behavior of wandering steps, we carry out a Monte Carlo simulation.[12,19,20] We use a square lattice model, and the lattice constant is set at $a = 1$. The boundary condition is periodic in the x direction and helical in the y direction in order to incorporate steps running in the x direction. We forbid two-dimensional nucleation and use solid-on-solid steps (the step position is a single-valued function of x). We choose the time increment for a diffusion trial Δt

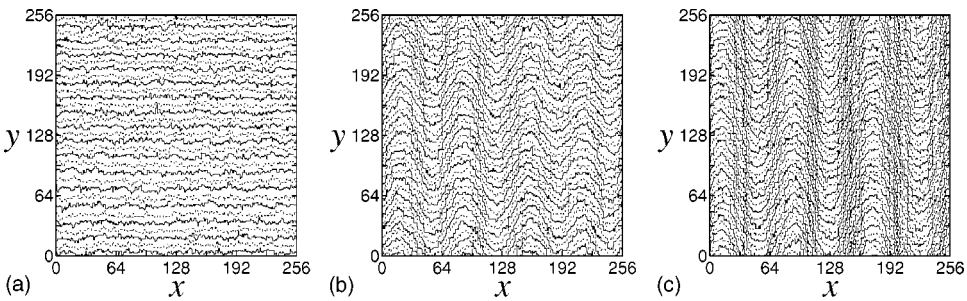

FIG. 2. Snapshots of the step wandering with (a) step-down drift at $t \approx 5.0 \times 10^5$, (b) step-up drift at $t \approx 2.5 \times 10^5$, and (c) step-up drift at $t \approx 12.4 \times 10^5$. The number of steps is 32 and the system size is 256×256.

$=1/4N_a$ (N_a is the number of adatoms) and the diffusion coefficient is chosen to be $D_\perp = 1$. The long-range step repulsion is taken into account in the y direction, but in the x direction, only the short-range repulsion is taken account by forbidding overlap of steps.

In a terrace A, an adatom on the site (i,j) moves to $(i \pm 1, j)$ with the probability 1/4 and to $(i, j \pm 1)$ with the probability $p_d(1 \pm Fa/2k_BT)/4$, where $p_d = D_\parallel / D_\perp (\leqslant 1)$ and F represent the anisotropy of the surface diffusion and the external force to induce the drift, respectively. In a terrace B, an adatom on the site (i,j) moves to $(i \pm 1, j)$ with the probability $p_d/4$ and to $(i, j \pm 1)$ with the probability $(1 \pm Fa/2k_BT)/4$. We use the permeable steps: adatoms diffuse over steps[12] 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

$$p_s = \left[1 + \exp\left(\frac{\Delta E_s + \Delta U - \phi}{k_B T} \right) \right]^{-1}, \tag{35}$$

where ΔE_s is the increment of the step energy and ϕ the potential gain by solidification. When there is no adatom on the top of a solid atom at the step position, melting occurs with the probability

$$p_m = \left[1 + \exp\left(\frac{\Delta E_s + \Delta U + \phi}{k_B T} \right) \right]^{-1}. \tag{36}$$

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

$$\frac{2\tilde{\beta}}{k_B T} = \sinh^2 \frac{\epsilon}{2K_B T}. \tag{37}$$

ΔU is the change of step-step interaction potential. For the long-range interaction in the y direction, we use the interaction potential $U = Al^{-2}$. The equilibrium adatom density of an isolated step satisfies the detailed balance $c^0_{eq} p_s = (1 - c^0_{eq}) p_m$ at a kink site where the perimeter length does not change by solidification or by melting, $\Delta E_s = 0$. Then, c^0_{eq} is given by[20]

$$c^0_{eq} = \frac{1}{1 + e^{\phi / k_B T}}. \tag{38}$$

The theoretical analysis is now compared with the results of Monte Carlo simulations. We study steps with an average distance $l = 8$ on a square lattice system of size 256×256 or 512×128. Length hereafter is measured in units of the lattice constant a, and time in units of $a^2/D_\perp$. The parameters are so chosen to be equilibrium adatom density $c^0_{eq} = 0.18$, step stiffness $\tilde{\beta}/k_BT = 0.13$, $D_\parallel = 0.5$, and $D_\perp = 1.0$. There is no extra energy barrier for the over-step diffusion. The kinetic coefficient is large enough so that the local equilibrium condition is valid. The strength of the repulsive potential $A/k_BT = 46$ is large enough to suppress step bunching in the following simulations.

In Fig. 2 we show snapshots of the step wandering under various drift forces; $f = 0.1$ for Fig. 2(a) and -0.1 for Figs. 2(b) and 2(c). Dotted lines represent the step S_A and solid lines represent the step S_B. We start the simulation with an equidistant train of straight steps. With step-down drift in Fig. 2(a) (upward drift in the figure), steps remain straight. With step-up drift in Figs. 2(b) and 2(c) step wandering occurs, in agreement with the linear stability analysis. Because the wandering is in phase, grooves appear parallel to the y axis.

Since $|fl| = 0.8$ is not very small, we have to use a general formula for the wavelength of the most unstable mode, and it is obtained to be $\lambda_{max} \approx 77$, in good agreement with the result $\lambda \approx 64$ in Fig. 2(b). There, the wandering amplitude (the average step fluctuation width) is $w \approx 14.5$, where w is defined by

$$w(t) = \frac{1}{N} \sum_{n=1}^{N} \sqrt{\frac{1}{L} \sum_{i=1}^{L} \left[y_n(i) - \frac{1}{L} \sum_{i}^{L} y_n(i) \right]^2}. \tag{39}$$

In a late stage shown in Fig. 2(c) the amplitude increases up to $w \approx 37.2$ when the wavelength of the grooves is about 85. Thus, the structure coarsens parallel as well as perpendicular to the steps.

Recently, Paulin and co-workers[16] studied the step wandering induced by the Ehrlich-Schwoebel effect in a conserved system. They found perpetual enhancement of the wandering amplitude as $w \sim t^\beta$ with $\beta \sim 1/2$, irrespective of the step repulsion, but the coarsening of the wavelength of grooves took place only with a step repulsion. Although we take account of the long-range step repulsion only in the y direction but not in the x direction as did Paulin *et al.*, the entropic repulsion may have caused an effective repulsion in the x direction and eventually the coarsening in our case, too.

In Fig. 3 open circles represent the time evolution of the wandering amplitude w for $f = -0.1$. The result is obtained

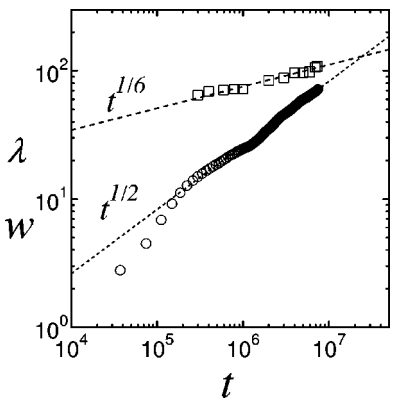

FIG. 3. Time evolution of the step width (○), $w \sim t^{1/2}$, and the groove wavelength (□), $\lambda \sim t^{1/6}$.

by averaging over ten runs of the size 512×128 with 16 steps. In an early stage ($t \leqslant 2 \times 10^5$), the step width increases rapidly. Then, the width enhancement slows down to $w \approx t^{1/2}$. The exponent is the same as the values obtained for the step wandering in other conserved systems.[13,14,16–18] The slowing down of the fluctuation amplification is attributed to the suppression of the diffusion current due to the narrowing of the terrace width.[16] The groove wavelength λ is obtained by counting the number of grooves for ten samples, and is depicted by open squares in Fig. 3. The slow increase as $\lambda \sim t^{\alpha}$ with $\alpha = 0.17 \pm 0.04$ is consistent with the one found with the use of a generalized version of Eq. (4).[16]

VI. SUMMARY AND DISCUSSION

In this paper, we studied the drift-induced step wandering on a vicinal face with an anisotropic surface diffusion whose orientation dependence alternates on consecutive terraces. The step-step interaction is shown to play an essential role for the step wandering, since it not only prevents steps from coalescing but also creates the difference Δc of the equilibrium adatom density. The imbalance of the diffusion current between different steps induced by Δc causes the step wandering. Thus the step repulsion mediates steps to establish the asymmetry in the diffusion field. Due to this asymmetry, the step wandering occurs with step-up drift. The in-phase wandering leads to the formation of straight grooves on a vicinal face, in accordance with other conserved systems.[13,14,16–18]

The present step wandering is unique since it happens only on a vicinal face. A steady state with only one isolated step pair is not possible in a conserved system. A simple analysis shows that, with weak evaporation, a step pair may be formed but a straight step pair is *stable with step-up drift*. Wandering instability occurs only with step-down drift. Therefore it is truly a many-body effect. In contrast, wandering instabilities known in ordinary systems [like those[21–23] of Si(111)] are essentially single-step instabilities. Wandering instabilities also occur on a vicinal face but the mechanism is the same for an isolated step and for a vicinal face.

Recently, in an experiment by Nielsen and co-workers[6] a dimpled specimen was used and step wandering on the Si(001) vicinal face was observed with the application of a direct electric current. Near the bottom of the dimple, where the inclination is very small, the step bunching occurs irrespective of the current direction.[24] The fluctuation of bunches with the step-up current is larger than that with the step-down current. On increasing the inclination, which means increasing the repulsive interaction, in-phase step wandering occurs and straight grooves parallel to the current appear with the step-up current. The step wandering was observed in a range of inclination angles between 0.08° and 0.5°. On the Si(001) vicinal face, the direction of the drift of adatoms is believed to be the same as that of the electric current,[7,8] and our results of step wandering under a step-up drift qualitatively agree with the experiment.[6]

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