Effect of two-dimensionality on step bunching on a Si(001) vicinal face

doi: 10.1143/JPSJ.75.043601

Effect of Two-dimensionality on Step Bunching on a Si(001) Vicinal Face

Masahide SATO[1] *, Makio UWAHA[2] and Yukio HIROSE[3]

[1] *Information Media Center of Kanazawa University, Kakuma-cho, Kanazawa 920-1192, Japan*
[2] *Department of Physics, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan*
[3] *Department of Computational Science, Kanazawa University, Kakuma-cho, Kanazawa 920-1192, Japan*

We study the effect of two-dimensionality on step bunching on a Si(001) vicinal face heated by direct electric current. When the anisotropy of the diffusion coefficient changes alternately on consecutive terraces like a Si(001) vicinal face, bunching occurs with the drift of adatoms. If the wandering fluctuation of step bunches is neglected as in the one-dimensional model, the bunching with step-down drift is faster than that with step-up drift in contradiction with experiment (Latyshev et al., Appl. Surf. Sci. **130**–**132**, 139 (1998)). In a two-dimensional model with a wide system width, the step bunches wander heavily with step-up drift, and the recombination of neighboring bunches occur more frequently than those with step-down drift. The bunching with step-up drift is accelerated and can be faster than that with step-down drift.

KEYWORDS: Step bunching, Step Wandering, Si(001)

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

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

The step instabilities are caused by drift of adatoms induced by the current. By taking account of the alternation of the anisotropic surface diffusion, the step instabilities are

*E-mail address: sato@cs.s.kanazawa-u.ac.jp

theoretically explained. If the repulsive interaction is strong such that the step bunching is suppressed, the step wandering occurs with step-up drift.[4] The motion of the steps is given by the solution of the nonlinear equation derived by Pierre-Louis and co-workers.[5,6] The step bunching occurs irrespective of the drift direction.[7–12] Since the current and the drift are in the same direction,[13,14] the results are consistent with the experiments.[1–3] In a one-dimensional step flow model,[12] the size of the bunches increases with time as t^{β} with $\beta \approx 0.4$, which roughly agrees with the experiment.[3] However, the growth rate with step-up drift is slower than that with step-down drift since terraces with fast diffusion along the current direction are dominant with step-down drift; this contradicts the experiment.[3] Since the model with alternating diffusion anisotropy has consistently explained the bunching and the wandering instabilities on the Si(001) vicinal face, this disagreement is a major obstacle in obtaining a unified understanding.

In the one-dimensional step flow models,[11,12] the motion of step bunches with step-down drift is similar to that with step-up drift, except for the time scale. In the Monte Carlo simulation, however, the step pattern is changed by the drift direction:[10,15] the step bunches with step-up drift wander more than those with step-down drift. A difference of this type in the two-dimensional step motion may solve the disagreement in the growth rate between the experiment[3] and the one-dimensional model.[11]

In this paper, we carry out Monte Carlo simulations and show that the growth rate of bunches can be reversed in the two-dimensional model. For simplicity, we use a square lattice model with the lattice constant $a = 1$. We consider the x-axis as parallel to the steps and y-axis in the down-hill direction. The boundary conditions are periodic in the x-direction and helical in the y-direction. Since the formation of two-dimensional islands and vacancies can be neglected in the experiments,[1–3] we forbid two-dimensional nucleation and use solid-on-solid steps, i.e., the step positions are single-valued functions of x.

In our simulation, we distinguish adatoms and solid atoms so that the lattice model in the continuum limit reduces to the standard step flow model.[11,12,15] We repeatedly select a solid atom at the step or an adatom on the terrace. We perform the diffusion and solidification trial for the adatom and melting trial for the solid atom. In the diffusion trial, the adatom hops to a neighboring site. The anisotropy of the diffusion coefficient and the drift of adatoms are taken into account in the hopping probability. With regard to $\mathrm{T_A}$, where the surface diffusion in the x-direction is faster, an adatom on site (i, j) moves to $(i \pm 1, j)$ with probability $1/4$ and to $(i, j \pm 1)$ with probability $p_{\mathrm{d}}(1 \pm Fa/2k_{\mathrm{B}}T)/4$, where $p_{\mathrm{d}}(< 1)$ is the ratio of the two diffusion coefficients. F is the force responsible for the drift. $F > 0$ represents the drift in the step-down direction. With regard to $\mathrm{T_B}$, where the surface diffusion in the y-direction is faster, an adatom on site (i, j) moves to $(i \pm 1, j)$ with probability $p_{\mathrm{d}}/4$ and to $(i, j \pm 1)$ with probability $(1 \pm Fa/2k_{\mathrm{B}}T)/4$. For a diffusion trial, the time increment is $\Delta t = 1/(4N_{\mathrm{a}})$, where

N_a is the number of adatoms so that the fast diffusion coefficient is unity.

If an adatom comes in contact with a step from the lower terrace after a diffusion trial, solidification occurs and the adatom is transferred to a solid atom with probability

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

On the Si(001) vicinal face, ΔE_s is complicated.[16] However, for simplicity, we neglect differences of step properties between S_A and S_B, and assume that the step energy is proportional to the step length: ΔE_s is given by $\Delta E_s = \epsilon \times$(the increment of the step perimeter due to the solidification), where ϵ is the half of the nearest-neighbor bonding enery, and ϕ is the decrement of the chemical potential by the solidification. The step stiffness $\tilde{\beta}$ is related to ϵ as

$$\frac{\tilde{\beta} a}{k_B T} = \frac{1}{2} \sinh^2 \frac{\epsilon}{k_B T}. \tag{2}$$

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

$$p_m = \left[1 + \exp\left(\frac{\Delta E_s + \phi}{k_B T}\right)\right]^{-1}. \tag{3}$$

There is no extra diffusion barrier over the steps: the steps are permeable. We neglect the long-range repulsive interaction between steps, but take into account a short-range repulsive interaction by forbidding the overlap of steps. Impingement of atoms and evaporation are absent.

Figures 1 and 2 represent snapshots of the step bunching. The system size is 256×256 and the number of steps is 64. The parameters are $\epsilon/k_B T = 0.5$, $\phi/k_B T = 1.5$, $Fa/2k_B T = \pm 0.08$, and $p_d = 0.25$. Initially, a few adatoms are present and the steps are equidistant. The dotted lines represent S_A steps and the solid lines represent S_B steps.

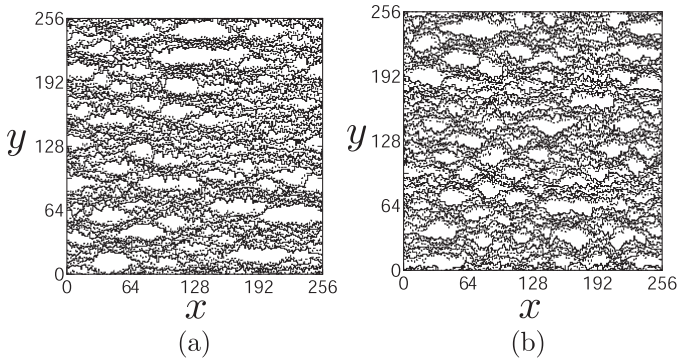

Fig. 1. Snapshots of step bunching at $t = 7.1 \times 10^2$ (a) with step-down drift and (b) step-up drift. The system size is 256×256 and the number of steps is 64.

The step bunching is suppressed by the strong repulsion and the step wandering occurs with the step-up drift.[15] In Fig. 1 the repulsion is absent and the step bunching occurs. In the initial stage, pairing of S_A and S_B occurs. The upper side step in a pair is S_A with step-up drift and S_B with step-down drift. Small bunches are formed by coalescence of step pairs. Since the stiffness is small, the bunches wander and connect with each other at many locations (Fig. 1). The figures may seem to indicate that the bunches with step-down drift are more straight than those with step-up drift.

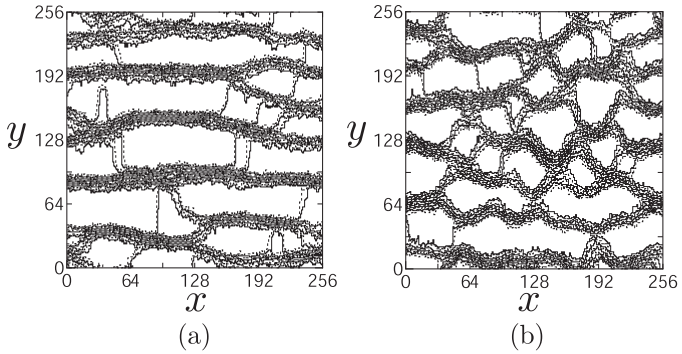

Fig. 2. Snapshots of step bunching (a) with step-down drift at $t = 3.6 \times 10^4$ and (b) step-up drift at $t = 3.5 \times 10^4$. The system size is 256×256 and the number of steps is 64.

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

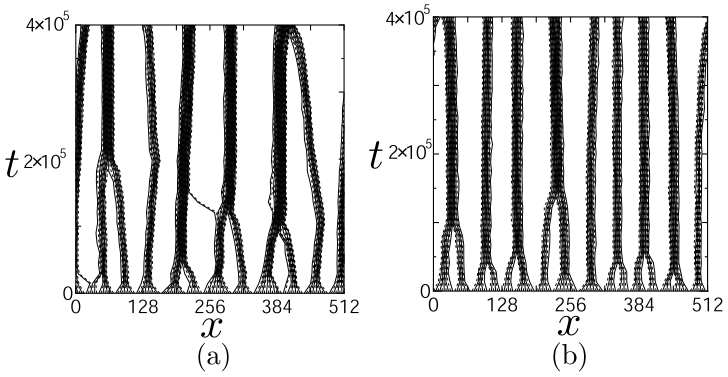

Fig. 3. Time evolution of averaged step positions (a) with step-down drift and (b) step-up drift. The system size is 8×512 and the number of steps is 128.

To investigate the effect of the wandering and recombination on the growth rate, we carry

out simulations with systems of two different widths. Figure 3 represents the time evolution of the average step positions in a narrow system of size 8×512 with 128 steps. The system is narrow to the extent that the bunches are straight and the crossing fluctuation with step-up drift is suppressed. The bunches grow due to the collisions of small bunches; this can be explained by the fluctuation of the terrace width. Since the long-range repulsive interaction is neglected in the simulation, we cannot compare the time scale with that in the one-dimensional model.[12] However, the time evolution of step bunches is similar to that in the one-dimensional model.[12]

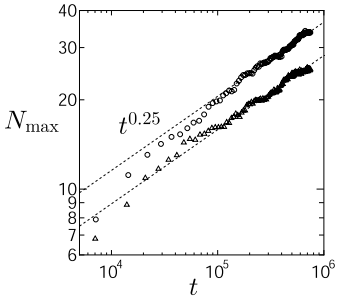

Fig. 4. Time evolution of the largest bunch size with step-up drift (△) and step-down drift (○). The system size is 8×512 and the number of steps is 128. The result is obtained by averaging over 20 runs.

In Figure 4, the number $N_{\max}$ of steps in the largest bunch at $x = 1$ is plotted as a function of time. The growth rate with step-up drift is slower than that with step-down drift, as in the one-dimensional model. The bunch size increases with time as t^{β} with $\beta \approx 0.25$.[17] The exponent differs from the value $\beta = 0.36 \sim 0.45$ in the one-dimensional model.[12] In the one dimensional model, the kinetic coefficient does not changes with an increase in the bunch size. Once the distance between the bunches fluctuates, the bunches begin to coalesce by the diffusion field. In the two-dimensional model, small fluctuations do not necessarily initiate the deterministic motion. With an increase in the buch size, the kink density extremely decreases and the kinetic coefficient becomes small. Because of the periodic boundary condition in the x-direction, time required for the bunch to appreciably shift the average position is more. The long waiting time is obvious from Fig.3. The retardation of the start of coalescence may cause a change in the growth exponent.

We carry out simulations in a much wider system: 1024×512. Figure 5 represents the time evolution of $N_{\max}$. The growth exponent is $\beta \approx 0.38$, which is larger than that in the narrow system and comparable with that of the one-dimensional system. As seen from Fig.2, steps crossing the large terraces connect step bunches. The steps cause the zipping of the bunches and trigger the coalescence of bunches, thereby preventing the retardation. In contrast to the one-dimensional model,[12] however, the growth of the bunch size with step-up drift is slightly

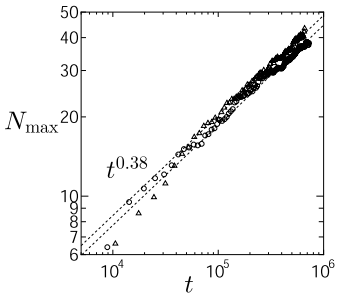

Fig. 5. Time evolution of the largest bunch size with step-up drift (△) and step-down drift (○). The system size is 1024×512 and the number of steps is 128. The result is obtained by averaging over 10 runs.

faster than that with step-down drift. With the step-up drift, the bunches wander and the recombination of bunches becomes more frequent. With the step-down drift, the step bunches are straight and the recombination of bunches becomes much less. As a result, the growth with step-up drift becomes faster than that with step-down drift. Thus, the slow diffusion in the y-direction is compensated by the efficient coalescence due to the wandering of bunches. Also, the fast diffusion in the x-direction with step-up drift facilitates the recombination of bunches. Consequently, the growth rate of bunches with step-up drift become faster than that with step-down drift.

The growth exponent $\beta \approx 0.38$ is slightly smaller than the experiment.[3] Our simulation model is still different from reality. The long-range step interaction is neglected, which certainly affects the exponent,[12] and the SOS condition is imposed on the steps, which tends to result in straight step pairs running in the y-direction on the terrace as seen in Fig.2(a). Such simplifications can also affect the exponent.

Remarks on the parameters adopted in the simulations are in order. On the Si(001) vicinal face, the step stiffness of S_A is larger than that of S_B. We have neglected the difference of the step stiffness and used the value $\beta a/k_B T = 0.14$, which is of the same order as that in the previous studies.[19,20] The difference in the step stiffness results in the difference in the kink density, which determines the kinetic coefficients. We have performed a series of simulations with smaller kinetic coefficients (reduction of the solidification probability) for the S_A. The result has shown that it helps the reversal of the growth rate of the bunch size.

On the Si(001) vicinal face, the difference of the diffusion barrier parallel to the dimer row from that perpendicular to the dimer row has been calculated as 0.3 eV.[18] Since the experiment[3] was carried out at $T = 1170^\circ$ C, the ratio p_d is estimated as $p_d \approx 0.09$. In our simulation, we used a larger value $p_d = 0.25$. By increasing the anisotropy of the diffusion coefficient, the wavelength of the in-phase step wandering becomes shorter[15] and the collision of the bunches occurs more frequently, which probably accelarate the step bunching. On the other hand, the one-dimensional model[12] predicts that the difference of the growth rate

with step-down drift and that with step-up drift increases with an increase in the diffusion anisotropy. Thus, it is not clear whether the increment in the diffusion anisotropy is responsible for the ease of reversal of the bunch size growth rate. This problem is currently begin studied.

Acknowledgments

This work was supported by the Grant-in-Aid for Scientific Research from the Japan Society for the Promotion of Science.

References

1) J.-F. Nielsen, M. S. Pettersen, and J. P. Pelz: Surf. Sci. **480** 2001) 84.
2) L. V. Litvin, A. B. Krasilnikov, and A. V. Latyshev: Surf. Sci. **244**(1991) L121.
3) A. V. Latyshev, L. V. Litvin, and A. L. Aseev: Appl. Surf. Sci. **130**–**132**(1998) 139.
4) M. Sato, M. Uwaha, Y. Saito, and Y. Hirose: Phys. Rev. B **67**(2003) 125408.
5) O. Pierre-Louis, C. Misbah, Y. Saito, J. Krug, and P. Politi: Phys. Rev. Lett. **80**(1998) 4221.
6) S. Paulin, F. Gillet, O. Pierre-Louis, and C. Misbah: Phys. Rev. Lett. **86**(2001) 5538.
7) S. Stoyanov: Jpn. J. Appl. Phys. **29**(1990) L659.
8) A. Natori, H. Fujimura, and H. Yasunaga: Jpn. J. Appl. Phys. **92**(1992) 1164.
9) A. Natori, H. Fujimura, and M. Fukuda: Appl. Surf. Sci. **60/61**(1992) 85.
10) M. Sato, M. Uwaha, and Y. Saito: J. Cryst. Growth **237**–**239**(2002) 43.
11) M. Sato, M. Uwaha, T. Mori, and Y. Hirose: J. Phys. Soc. Jpn **72**(2003) 2850.
12) M. Sato, T. Mori, M. Uwaha, and Y. Hirose: J. Phys. Soc. Jpn **73**(2004) 1827.
13) M. Ichikawa and T. Doi: Appl. Phys. Lett. **60**(1992) 1082.
14) J.-J. Métois, J.-C. Heyraud, and A. Pimpinelli: Surf. Sci. **420**(1999) 250.
15) M. Sato, M. Uwaha, Y. Saito, and Y. Hirose: Phys. Rev. B **67**(2003) 125408.
16) B. S. Swartzentruber, Y.-W. Mo, R. Kariotis, M. G. Lagally, and M. B. Webb: Phys. Rev. Lett. **65**(1990) 1913.
17) On account of the limited size of our simulation, it is difficult to define the bunch size. We regard a step pair as being contained in the bunch if the distance between the step pair and the bunch is smaller than a prescribed value. The obtained exponent depends on this value, though not very sensitively.
18) S. Jeong and A. Oshiyama: Phys. Rev. Lett. **79**(1997) 4425.
19) N. C. Bartelt, R. M. Tromp, and E. D. Williams: Phys. Rev. Lett. **73**(1994) 1656.
20) N. Akutsu and Y. Akutsu: Phys. Rev. B **57**(1998) R4233.