Effect of impingement and evaporation on drift-induced step instabilities on Si(1 1 1) vicinal face near transition temperature

Effect of Impingement and Evaporation on Drift-Induced Step Instabilities on Si(111) Vicinal Face near Transition Temperature

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Abstract

Bearing the Si(111) vicinal face in mind, we study the effect of impingement and evaporation on drift-induced step instabilities. On a Si(111) face, transition between 1×1 structure and 7×7 structure occurs at 860°C. On the vicinal face near the transition temperature, the two structures coexist: the 1×1 structure is at the lower side of step and the 7×7 structure is at the upper side. On the 1×1 structure, the diffusion coefficient is larger than that on the 7×7 structure. When the difference in the diffusion coefficients is taken into account, step bunching occurs with drift of adatoms. In a conserved system with fast drift, separation and coalescence of steps occur repeatedly, and the bunches grow gradually. The motion of bunches changes when the impingement or evaporation is present. With the impingement, the separation of steps is suppressed and the bunches grow via coalescence of small ones with step-down drift, while the separation is more frequent than that in conserved system with step-up drift. With the evaporation, the relation is the opposite.

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I. INTRODUCTION

Si(111) surface covered with 1×1 structure is reconstructed and the 7×7 structure appears when temperature is lower than transition temperature (≈ 860°C). On a vicinal face, the 7×7 structure appears from the upper side of the step edge [1], and the 1×1 structure and the 7×7 structure coexist in a terrace near the transition temperature. On the 1×1 structure, the product of the diffusion coefficient and the equilibrium adatom density is larger than that on the 7×7 structure [2].

Previously, bearing the Si(111) vicinal face with two structures in mind, we studied the possibility of the step bunching on a vicinal face [3]. We took account of the difference in the diffusion coefficients, and showed that the step bunching occurs irrespective of the drift direction. With step-down drift, the region with the 1×1 structure is more dominant than that with the 7×7 structure, and the relation is the opposite with step-up drift. With slow drift, the bunches grow via coalescence of small bunches, while the separation of steps from bunches repeatedly occurs with fast drift. In the previous study [3], we neglected the impingement and the evaporation of adatoms, but they may change the motion of steps.

In this paper, we study the effect of the impingement and the evaporation on the drift-induced step bunching by Monte Carlo simulation. In Sec. II, we introduce the model, and show the results in Sec. III. In Sec. IV, we summarize the results and carry out brief discussions.

II. MODEL

We use a very simple model [3, 4], where the difference in the diffusion coefficients is taken into account. We consider a square lattice model with the lattice constant $a = 1$. The phase boundaries of the two structures and the steps are parallel to the x-axis on average and the step-down direction is the y-direction. We use the periodic boundary condition in the x-direction and the helical boundary condition in the y-direction.

At the phase boundary, adatoms are adsorbed when the boundary advances, and desorbed when the boundary recedes, which are similar to the steps. Thus, we treat the boundaries as steps. We take account of the short-range repulsion between a step and a boundary to forbid overlapping, but neglect the long-range repulsion.

In the experiment [2], the product of the equilibrium adatom density and the diffusion coefficient on the 1×1 structure is larger than that on that 7×7 structure. In the simulation, we assume that the equilibrium adatom densities are the same on the two structures, and take account of the difference in the diffusion coefficients.

The model we use is similar to that in the previous studies [3–9]. In the model, solid atoms and adatoms are distinguished. Active atoms are adatoms, solid atoms at the steps and that at the phase-boundary. We randomly choose an active atom from them. When an adatom is chosen, the evaporation trial or hopping to one of the nearest neighboring sites is tried.

On the region with fast diffusion coefficient, where the diffusion coefficient is D_1, an adatom on a site (i,j) hops to $(i\pm1,j)$ with the hopping probability $D_1/4$, and to $(i,j\pm1)$ with the probability $D_1(1\pm F_{\rm d}/k_{\rm B}T)/4$, where $F_{\rm d}$ is the force to cause the drift of adatoms. On the region with slow diffusion coefficient, D_1 is replaced to D_2 which is smaller than D_1. The time increase Δt in a hopping trial is $\Delta t = 1/(4D_1N_{\rm a})$, where $N_{\rm a}$ is the number of adatoms. The evaporation ratio per unit time is $p_{\rm e} = \Delta t/\tau$, where τ is the lifetime of adatoms. After a few diffusion trials, the impingement of adatoms is tried with the impingement rate F.

After the diffusion trial, if the adatom attaches to a solid atom from the lower side, a solidification trial is successively carried out. When a solid atom is chosen, a melting trial is carried out if an adatom is absent on the top of the solid atom. The probability p_+ of solidification and that p_- of melting are given by [5]

$$p_\pm = \left[1+\exp\left(\frac{\Delta E_{\rm s}\pm\phi}{k_{\rm B}T}\right)\right]^{-1}, \tag{1}$$

where $\Delta E_{\rm s} = \epsilon\times$ (the increase of the step perimeter). ϵ is the half of the step energy and ϕ is the decrease of the chemical potential by solidification.

III. RESULTS OF SIMULATION

Figure 1 shows images of step bunching without the evaporation and the impingement. The parameters are $\epsilon/k_{\rm B}T = 0.8$ and $\phi/k_{\rm B}T = 1.5$. The force to cause the drift is $F_{\rm d}a/k_{\rm B}T = 0.3$ with step-down drift and $F_{\rm d}a/k_{\rm B}T = -0.4$ with step-up drift. The number of steps is

16 and the system size is $L_x \times L_y = 256 \times 256$. Irrespective of the drift direction, the step bunching occurs. Dark region represents the region with fast diffusion coefficient, and light region represents the region with slow diffusion coefficient. The type of dominant region changes with the drift direction: the region with slow diffusion is dominant with step-up drift and that with fast diffusion is dominant with step-down drift. Step bunches with step-down drift fluctuate largely (Fig. 1(a)) and recombinate, while the bunches with step-up drift are straight (Fig. 1(b)).

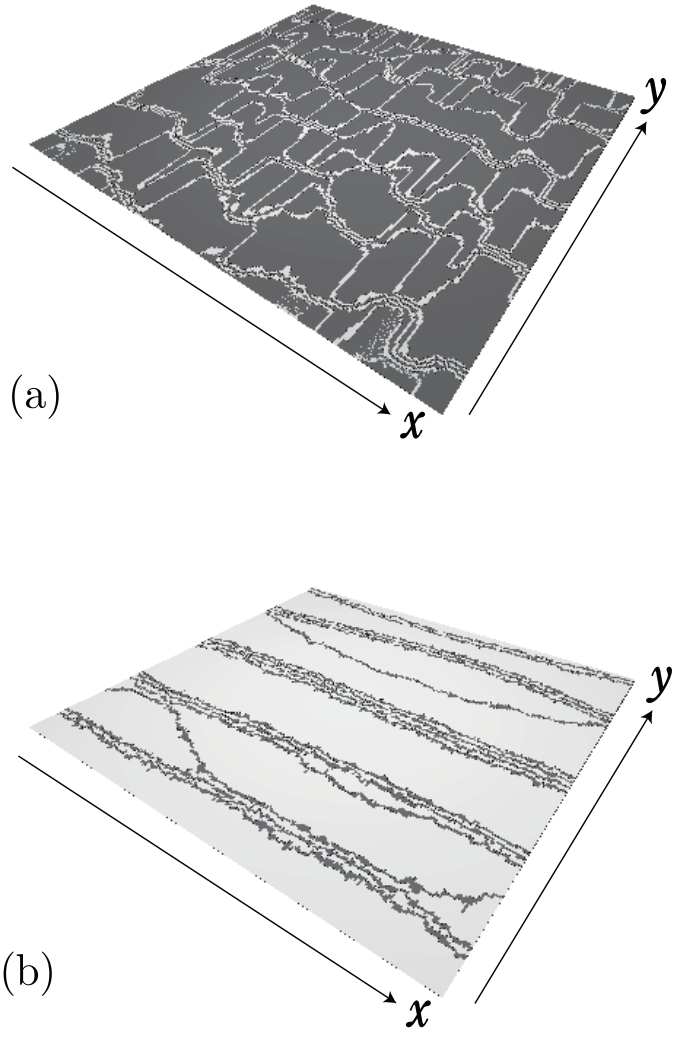

FIG. 1: Snapshots of step bunching in a conserved system (a) with step-down drift and (b) with step-up drift.

Figure 2 shows the time evolution of average step positions. To suppress the fluctuation of bunches, we use a narrow system, $L_x \times L_y = 16 \times 512$. Other parameters are the same as those in Fig. 1. Since the step and the boundary move as a pair, we shows only the step position in Fig. 2. The bunches with step-down drift grow faster than that with step-up drift. (See the difference in the time scale between Fig 2(a) and Fig 2(b).) In an early stage, the bunches grow via coalescence of small ones and the single steps does not appear on large terraces. When the bunch size is large in a later stage, the separation of steps repeatedly occurs. The separated step recedes with step-down drift and advances with step-up drift. The velocity of the separated step with step-down drift is much faster than that with step-up drift.

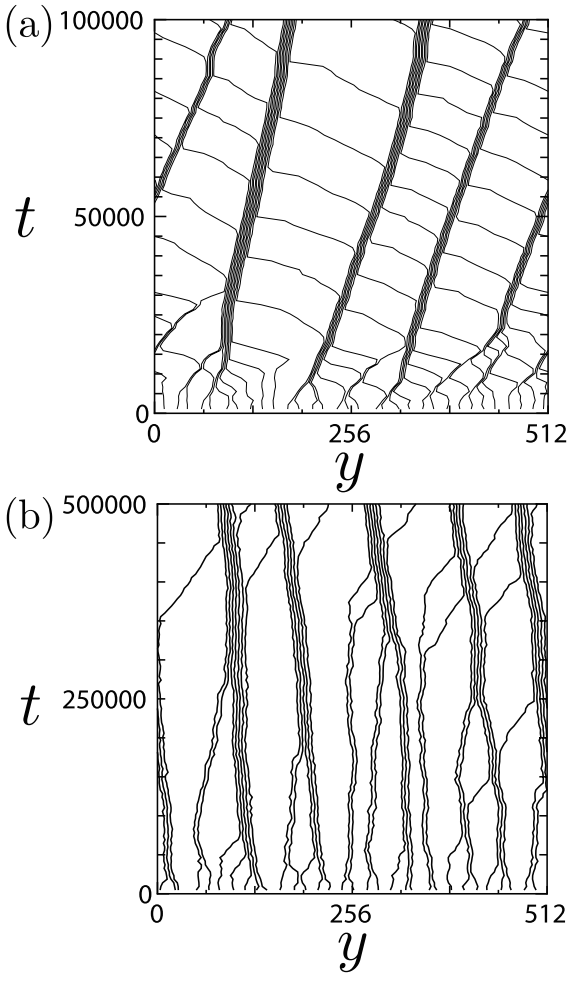

FIG. 2: Time evolution of average step positions in a conserved system (a) with step-down drift and (b) with step-up drift.

The difference in the step motion is related to that of the distribution of adatom density.

Figure 3 shows the relation between the distribution of adatom density and the positions of bunches in a conserved system. On the large terrace, the region with fast diffusion is dominant with step-down drift. The average drift velocity on the large terrace is larger than that in bunches. The adatoms are accumulated in bunches (Fig. 3(a)). The adatom density on large terrace is smaller than the equilibrium adatom density. Thus, if the step separate from the bunches, the step is in the region with low adatom density and recedes. With step-up drift, the situation is the opposite: the region with slow diffusion is dominant on large terrace. The adatom density on the large terraces is larger than the equilibrium value, and the separated step advances. From Fig. 3(b), however, the difference in the adatom density is small. Thus, the step velocity with step-up drift is smaller than that with step-down drift.

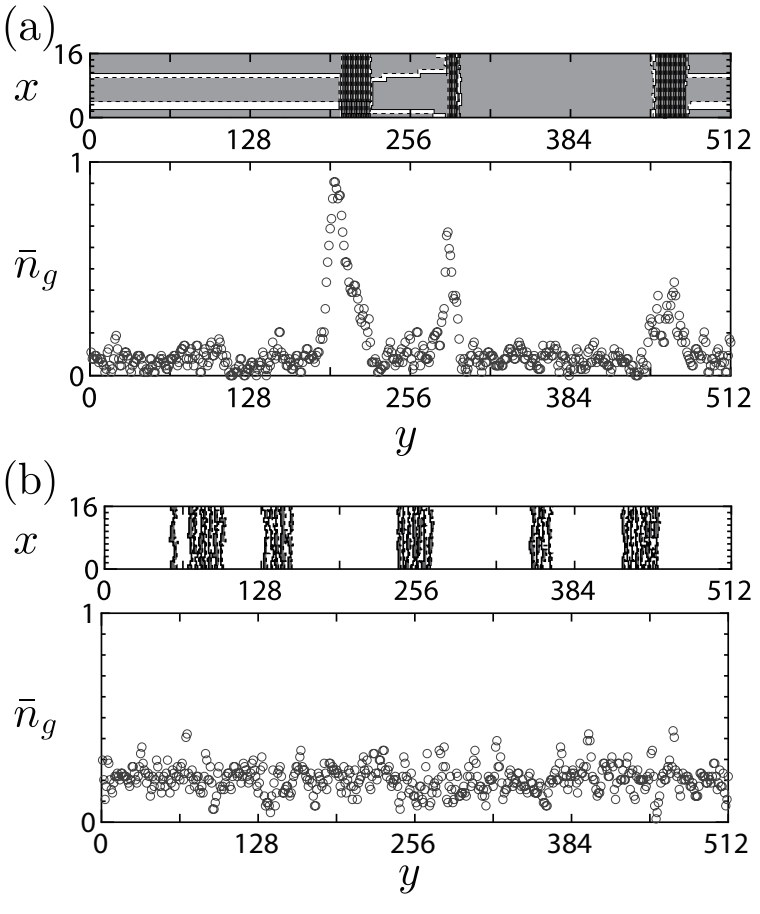

FIG. 3: Relation of step position and adatom density in a conserved system (a) with step-down drift and (b) with step-up drift.

The impingement and the evaporation change the formation of bunches. Figure 4 shows the time evolution of average step positions in growth. The impingement rate is $f = 10^{-4}$.

With step-down drift (Fig. 4(a)), the separation of steps is suppressed, and with step-up drift (Fig. 4(b)), the separation is more frequent than that in the conserved system.

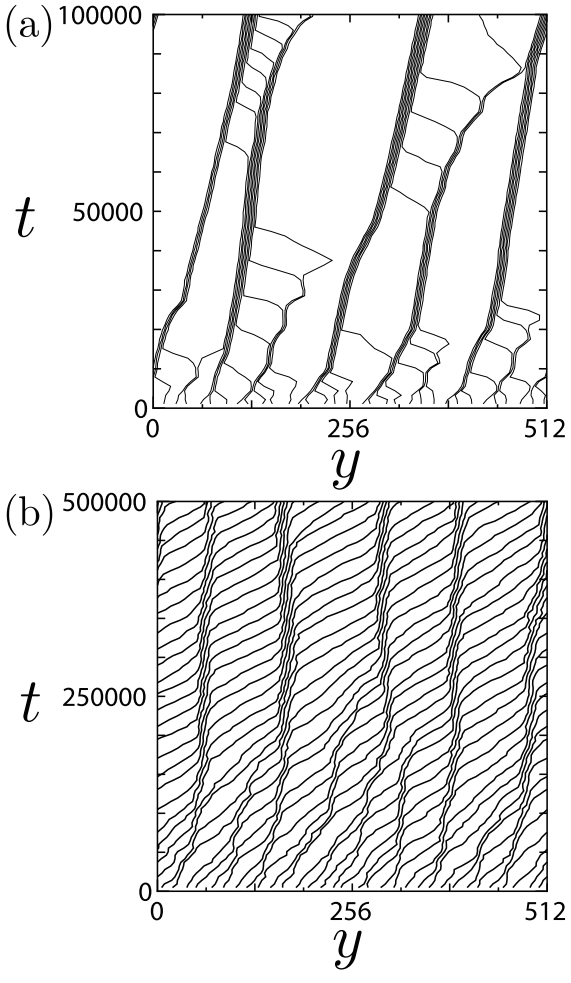

FIG. 4: Time evolution of step positions in growth (a) with step-down drift and (b) with step-up drift.

The change of the frequency of separation of steps is explained by the change the distribution of adatom density. With the impingement of atoms, the adatom density on the large terrace increases. When the drift is in the step-down direction, the separated step releases atoms and recedes. The increase of the adatom density by the impingement prevents the release of adatoms by step receding. Then, the frequency of separation decreases. When the drift is in the step-up direction, the separated step absorbs adatoms and advances. The increase of adatom density increases the absorption of adatoms, the step is enhanced to advance and the frequency of separation increases. The increase of adatom density is so large that the separation of step is more frequent than that in conserved system as shown

in Fig. 4(b).

With the evaporation of adatoms, the relation is the opposite. Figure 5 shows the time evolution of step position in sublimation with $\tau = 1024$. The evaporation decreases the adatom density on large terrace. With step-down drift (Fig 5(a)), the release of adatoms from the separated step is enhanced, and the frequency of the separation of step increases. With step-up drift (Fig 5(b)), the adsorption of adatoms is suppressed and the frequency of separation of steps decreases.

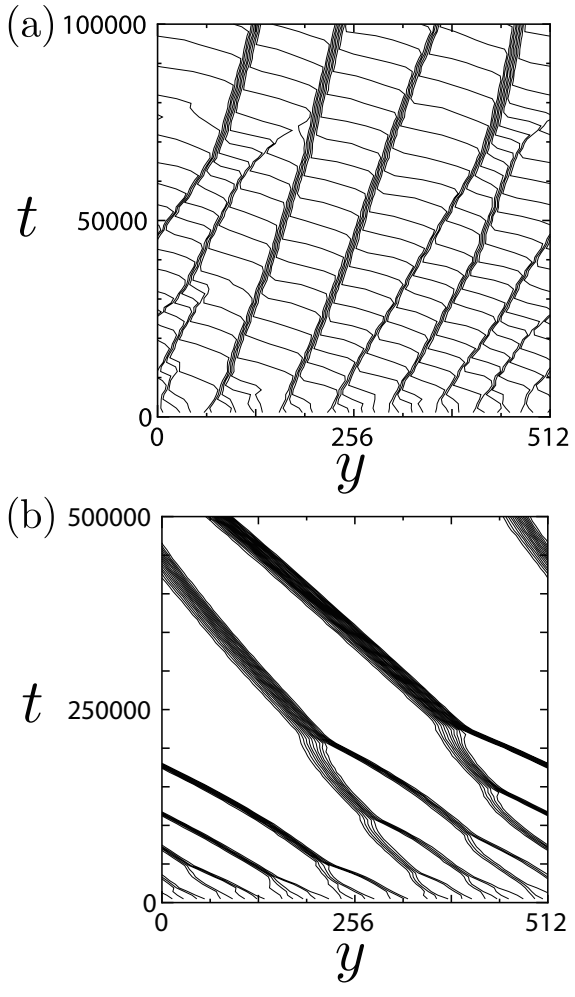

FIG. 5: Time evolution of step positions in sublimation (a) with step-down drift and (b) with step-up drift.

IV. SUMMARY AND DISCUSSION

In this paper, bearing the Si(111) vicinal face near the transition temperature in mind, we studied the effect of the impingement and the evaporation of adatoms on the step bunching. In the conserved system, in which the evaporation and the impingement are neglected, the step bunching occurs irrespective of drift direction. With increasing the bunch size, the gap in the adatom density between on terrace and in bunch is formed. With step-down drift (in Fig. 3(a)), the adatom density in bunch is smaller than the equilibrium value, $c_{\rm eq} = 0.18$. Thus, the step separates from a bunch, the adatoms is released from the step to increase the adatom density on the terrace and the step recedes. With step-up drift, the situation is the opposite.

In growth, the adatom density on large terrace increases. With step-down drift, the increase of the adatom density suppresses the release of atoms from the separated step. The step recedes slowly and the frequency of the separation decreases. With step-up drift, the increase of the adatom density enhances the adsorption of adatoms at the separated step. Then, the step advances fast and the frequency of separation increases. In sublimation, the relation is the opposite: the separation with step-down drift is more frequent than that in conserved system, and that with step-up drift is less frequent. Both in conserved system and in the system with the impingement, the bunches with step-down drift is more tight than those with step-up drift, but in the system with the evaporation, the bunches with step-up drift seems to be as tight as those with step-down drift.

On the Si(111) vicinal face, the 1×1 structure and 7×7 structure coexist near 860° C. Since the temperature is low, the surface diffusion length is probably very long, and the effect of the evaporation is weak. However, the effect may be observed if the experiment similar to Ref [10] is carried out. The experiment is desirable.

Acknowledgments

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[1] N. Osakabe, Y. Tanishsiro, K. Yagi, and G. Honjo: Surf. Sci. **109** (1981) 3682.

[2] H. Hibino, C.-W. Hu, T. Ogino and I. S. T. Tsong: Phys. Rev. B **63** (2001) 245401.

[3] K. Ikawa, M. Sato and M. Uwaha, J. Phys. Soc. Jpn. **76** (2007) 06402.

[4] R. Kato, M. Uwaha, and Y. Saito: Surf. Sci. **550** (2004) 149.

[5] Y. Saito and M. Uwaha: Phys. Rev. B **49** (1994) 10677.

[6] R. Kato, M. Uwaha, Y. Saito, and H. Hibino: Surf. Sci. **522** (2003) 64.

[7] M. Sato, M. Uwaha, Y. Saito, and Y. Hirose: Phys. Rev. B **65** (2002) 245247.

[8] M. Sato, M. Uwaha, Y. Saito, and Y. Hirose: Phys. Rev. B **67** (2003) 125408.

[9] M. Sato, M. Uwaha, and Y. Saito: J. Cryst. Growth **275/1-2** (2005) e129.

[10] J.J. M'etois, J. C. Heyraud and S. Stoyanov: Surf. Sci. **486** (2001) 95.

Figure Captions

Figure 1

Snapshots of step bunching in a conserved system (a) with step-down drift and (b) with step-up drift.

Figure 2

Time evolution of average step positions in a conserved system (a) with step-down drift and (b) with step-up drift.

Figure 3

Relation of step position and adatom density in a conserved system (a) with step-down drift and (b) with step-up drift.

Figure 4

Time evolution of step positions in growth (a) with step-down drift and (b) with step-up drift.

Figure 5

Time evolution of step positions in sublimation (a) with step-down drift and (b) with step-up drift.

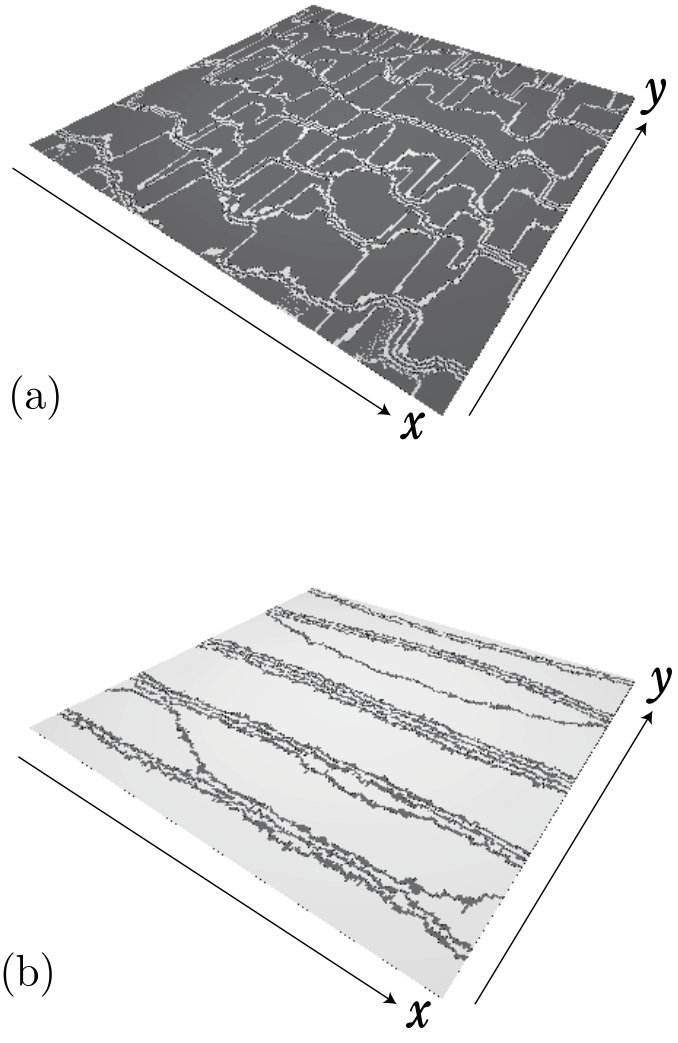

Fig. 1: K. Ikawa and M. Sato

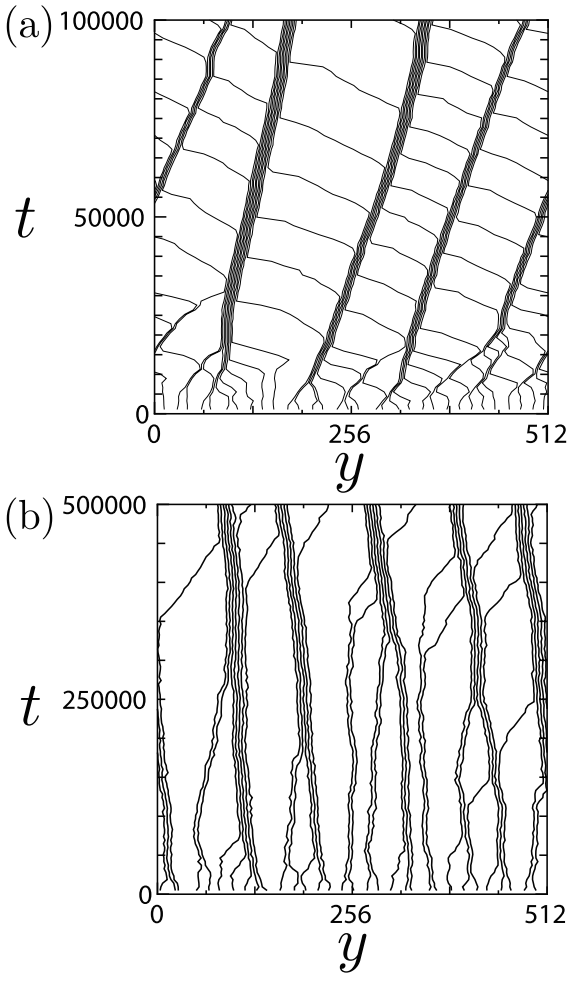

Fig. 2: K. Ikawa and M. Sato

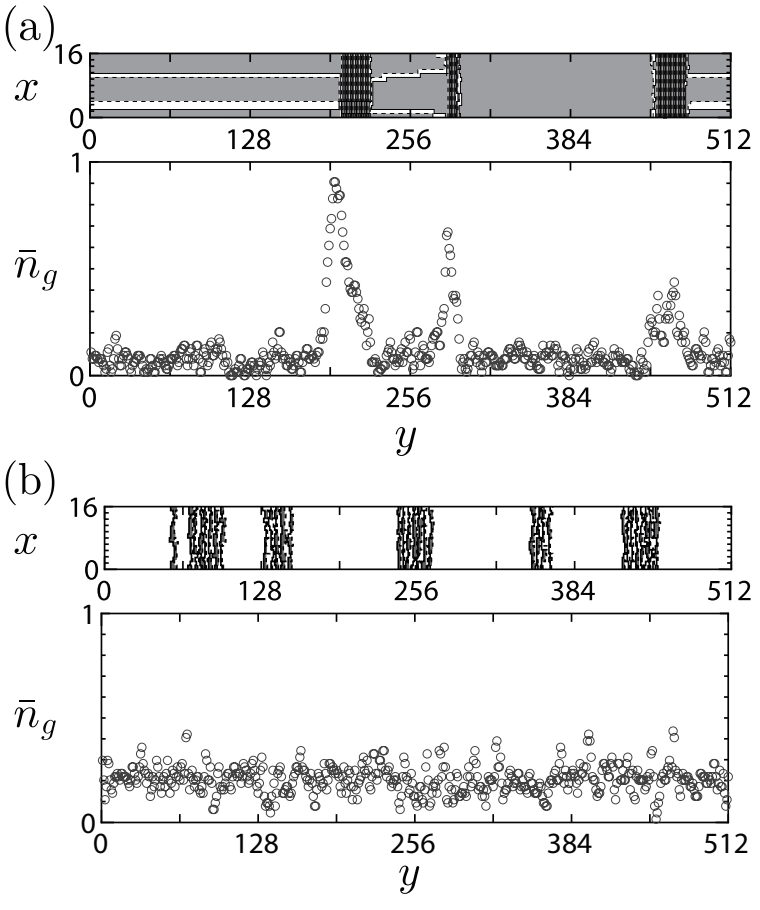

Fig. 3: K. Ikawa and M. Sato

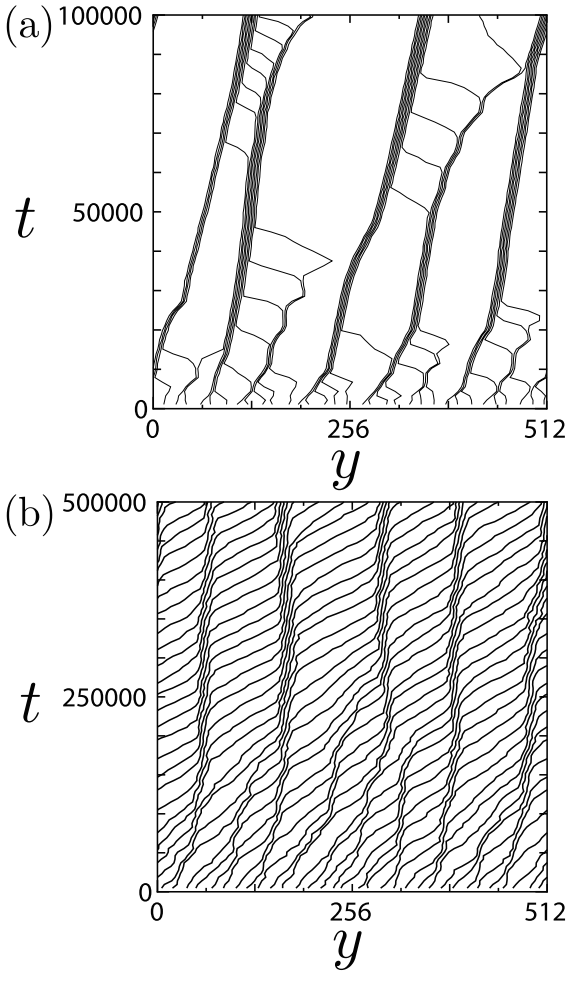

Fig. 4: K. Ikawa and M. Sato

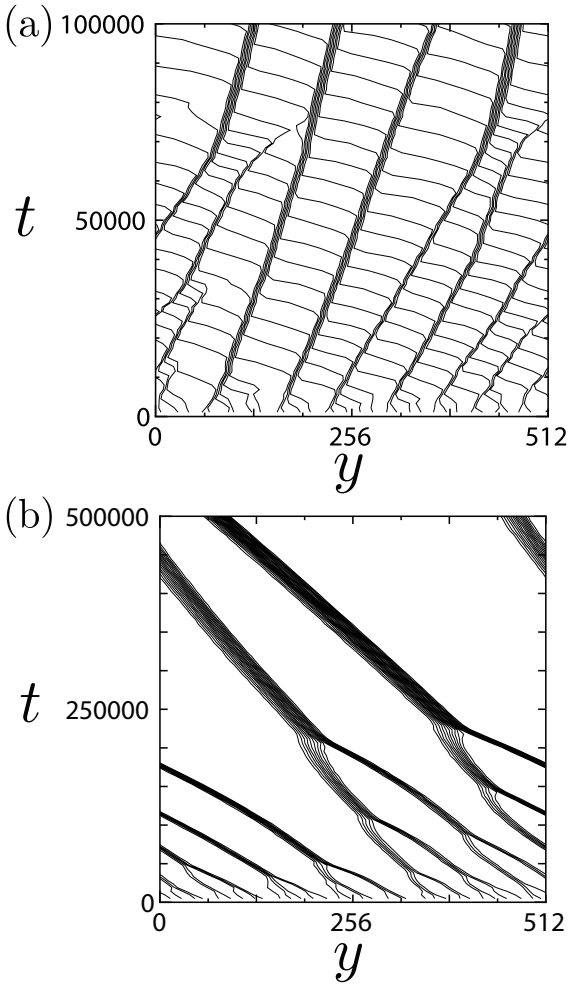

Fig. 5: K. Ikawa and M. Sato