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Step Instabilities on Si(111) Vicinal Face near $1 \times 1 \leftrightarrow 7 \times 7$ Transition Temperature during sublimation

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On a Si(111) vicinal face near the structural transition temperature (860 °C), the 7×7 structure and 1×1 structure coexist on a terrace. The 7×7 structure is on the upper side of steps and the 1×1 structure is on the lower side of steps. The diffusion coefficient on the 1×1 structure is larger than that on the 7×7 structure. In this paper, taking account of the difference in the diffusion coefficient, we study the possibility of step instabilities, step wandering and step bunching, occurring during sublimation.

KEYWORDS: Si(111) vicinal face, step bunching, step wandering, Kuramoto-Sivashinsky equation

1. Introduction

At high temperatures, the Si(111) surface is covered with the 1×1 structure. When the temperature decreases to lower than the structural transition temperature (860 °C), the 7×7 structure appears on the surface. Near the structural transition temperature, both these structures coexist on a terrace.¹⁾

On the vicinal face near the structural transition temperature, the 7×7 structure spreads from the upper side of steps. The 7×7 structure is present on the upper side of steps and the 1×1 structure is present on the lower side [Fig. 1(a)]. From a previous experiment,²⁾ the product of the diffusion coefficient D_s and the equilibrium adatom density c_{eq} on the 7×7 structure is smaller than that on the 1×1 structure.

Step wandering and step bunching have been observed³⁻⁷⁾ on the Si(111) vicinal face at high temperatures and have been theoretically studied.⁸⁻¹⁴⁾ Hibino et al. observed step wandering near the structural transition temperature on a growing vicinal face.¹⁵⁾ On the vicinal face, grooves perpendicular to the step are formed by the in-phase step wandering. Kato et al. theoretically studied the wandering.^{16,17)} They neglected the difference in the equilibrium adatom density, and took account of the difference in the diffusion coefficient. According to a linear stability analysis, the vicinal face is unstable against step wandering. Owing to in-phase step wandering, grooves perpendicular to the steps are formed according to the results of a Monte Carlo simulation.

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Hibino et al. added a direct electric current parallel to the step and observed step wandering on the growing vicinal face.¹⁵⁾ The grooves are tilted by the direct electric current. On Si surfaces, the direct electric current is considered to induce the drift of adatoms parallel to the current.³⁾ In a theoretical study, we carried out a linear stability analysis and Monte Carlo simulations, and showed that the tilting of grooves is formed by the drift of adatoms.

In experimental¹⁵⁾ and theoretical studies,^{16–18)} the instabilities of step in growth have been studied, but the effect of evaporation has not been sufficiently studied theoretically. In this paper, considering the Si(111) vicinal face with the 1×1 and 7×7 structures, we study the possibility of step bunching and step wandering occurring during sublimation.

In § 2 we describe the model we used. In § 3, taking account of the differences in the diffusion coefficient, we carry out stability analysis. In § 4, we carry out Monte Carlo simulations. In § 5, we summarize the results and give a brief discussion.

2. Model

We consider a vicinal face, where the x -direction is parallel to the edge of each step and the y -direction is in the step-down direction of the steps (Fig. 1(a)). When we neglect the impingement of atoms and the drift of adatoms, the diffusion equation, which the adatom density $c(\mathbf{r}, t)$ obeys, is given by

$$\frac{\partial c(\mathbf{r}, t)}{\partial t} = D_s(\mathbf{r}) \nabla^2 c(\mathbf{r}, t) - \frac{1}{\tau} c(\mathbf{r}, t), \quad (1)$$

where τ is the lifetime of adatoms and $D_s(\mathbf{r})$ is the local diffusion coefficient. $D_s(\mathbf{r}) = D_1$ on the 1×1 structure on the lower side of a step and $D_s(\mathbf{r}) = D_2$ on the 7×7 structure on the upper side of a step. Since the diffusion coefficient on the 1×1 structure is larger than that on the 7×7 structure,²⁾ we assume that D_1 is larger than D_2 . For simplicity, we assume that the evaporation rate on the 1×1 structure is the same as that on the 7×7 structure.

In an experiment,¹⁹⁾ it was observed that the structural boundary advances with the absorption of adatoms and recedes with the release of adatoms, similar to the motion of the step. Then, we treat the structural boundary as a step (Fig. 1(b)). When the boundary moves, the number of adatoms adsorbed by the boundary is much smaller than that adsorbed by the step.²⁰⁾ However, following Kato et al.,^{17,18)} we neglect the difference in properties between the step and boundary.

At steps and boundaries, we assume that the adatom densities are in equilibrium:

$$c|_{s(b)} = c_{\text{eq}}^{s(b)}, \quad (2)$$

where $s(b)$ indicates the step (boundary). The equilibrium adatom density at a step c_{eq}^s and that at the structural boundary c_{eq}^b are given by

$$c_{\text{eq}}^{s(b)} = c_{\text{eq}}^0 \left(1 + \frac{\Omega \tilde{\beta} \kappa^{s(b)}}{k_B T} \right), \quad (3)$$

Fig. 1. (a) Si(111) vicinal face near $1 \times 1 \leftrightarrow 7 \times 7$ structural transition temperature and (b) our model in which structural boundaries are treated as steps.

where c_{eq}^0 is the equilibrium adatom density at an isolated step, Ω is the atomic area, $\tilde{\beta}$ is the step stiffness, and $\kappa^{s(b)}$ is the curvature. In eq. (3), the repulsive interaction between a step and a boundary is neglected.

By solving the diffusion equation, eq. (1) with the boundary conditions, eq. (2) in the quasi-static approximation ($\partial c / \partial t = 0$), the velocity of the steps V_s and that of boundaries V_b are given by

$$V_s = \Omega(j|_{s-} - j|_{s+}) \cdot n_s, \quad (4)$$

$$V_b = \Omega(j|_{b-} - j|_{b+}) \cdot n_b, \quad (5)$$

where $+$ ($-$) indicates the lower (upper) side of the steps and boundaries, and $n_{s(b)}$ is the normal vector of the step (structural boundary) in the stepward direction of the step.

3. Linear Stability Analysis

We assume that the steps and boundaries are straight. When the steps and boundaries are equidistant with distance l , the diffusion equation in the quasi-static approximation is given by

$$D_s \frac{d^2 c}{dy^2} - \frac{1}{\tau} c = 0. \quad (6)$$

By solving eq. (6) with $c|_{s(b)} = c_{\text{eq}}^0$, the adatom density is obtained. From eqs. (4) and (5), the velocity of the step V_s^0 and that of the boundary V_b^0 are given by

$$\begin{aligned} V_s^0 &= V_b^0 \\ &= -\frac{\Omega D_1}{x_1} \tanh \frac{l}{2x_1} - \frac{\Omega D_2}{x_2} \tanh \frac{l}{2x_2}, \end{aligned} \quad (7)$$

where the surface diffusion lengths, x_1 and x_2 , are given by $x_1 = \sqrt{D_1\tau}$ and $x_2 = \sqrt{D_2\tau}$. The steps and boundaries recede with the same velocity.

We assume a small fluctuation of the distance between each step and boundary, and study the stability of the array of equidistant pairs consisting of a step and boundary. When the width with the diffusion coefficient D_1 is $l + \delta l$ and that with the diffusion coefficient D_2 is $l - \delta l$, the change of step velocity δV_1 and that of boundary velocity δV_2 are given by

$$\delta V_1 = \delta V_2 = \frac{\Omega}{2\tau} \left(\cosh^{-2} \frac{l}{2x_1} - \cosh^{-2} \frac{l}{2x_2} \right) \delta l. \quad (8)$$

Since we assume that D_1 is larger than D_2 ,

$$\left(\cosh^{-2} \frac{l}{2x_1} - \cosh^{-2} \frac{l}{2x_2} \right) > 0. \quad (9)$$

If δl is negative, the region with a large evaporation rate decreases. The average evaporation becomes small and the velocity at which the steps and boundaries recede decreases. In the opposite case, the average evaporation rate becomes large and the receding velocity increases. Irrespective of the sign of δl , the change δV_1 of velocity of step is the same as that δV_2 of velocity of boundary. Thus, the pairing of boundary and step does not occur.

If the surface diffusion lengths, x_1 and x_2 are smaller than the distance between a step and a boundary, we can treat them as isolated. We consider an isolated step and study the stability in terms of step wandering. When the fluctuation of a step is given by $\zeta = \zeta_0 e^{iqx + \omega t}$, the adatom density is changed by the fluctuation and is given by $c(x, y) = c_0(y) + c_1(y) e^{iqx + \omega t}$. The diffusion equation for $c_1(y)$ is given by

$$D_s \left(\frac{d^2 c_1}{dy^2} - q^2 c_1 \right) - \frac{1}{\tau} c_1 = 0, \quad (10)$$

where D_s is D_2 on the upper side of the step and D_1 on the lower side. From eq. (3), the boundary condition is given by

$$\left. \frac{dc_0}{dy} \right|_{y=0} \zeta_0 + c_1|_{y=0} = \frac{\Omega c_{eq}^0}{k_B T} q^2 \zeta_0. \quad (11)$$

By solving the diffusion equation, eq. (10) with the boundary condition, eq. (11), the adatom density is obtained. From eq. (4), the rate of amplification of the fluctuation is given by

$$\begin{aligned} \omega = & \frac{\Omega c_{eq}^0}{\tau} \left(\sqrt{1 + (qx_2)^2} - \sqrt{1 + (qx_1)^2} \right) \\ & - \frac{\tilde{\Omega} \beta c_{eq}^0}{k_B T} q^2 \frac{D_2}{x_2} \sqrt{1 + (qx_2)^2} \\ & - \frac{\tilde{\Omega} \beta c_{eq}^0}{k_B T} q^2 \frac{D_1}{x_1} \sqrt{1 + (qx_1)^2}. \end{aligned} \quad (12)$$

When the wavelength of the fluctuation is longer than x_1 and x_2 , eq. (12) is expressed as

$$\omega = \alpha_s q^2 + \beta_s q^4, \quad (13)$$

where α_s and β_s are given by

$$\alpha_s = \Omega c_{\text{eq}}^0 \left[\frac{(D_2 - D_1)}{2} - \frac{\tilde{\beta}}{k_B T} \left(\frac{D_2}{x_2} + \frac{D_1}{x_1} \right) \right], \quad (14)$$

$$\beta_s = -\frac{\tilde{\Omega}\beta c_{\text{eq}}^0}{2k_B T} (D_1 x_1 + D_2 x_2). \quad (15)$$

Since α_s and β_s are negative, the step is stable against the fluctuation. For an isolated phase boundary, the amplification rate is expressed by

$$\omega = \alpha_b q^2 + \beta_b q^4, \quad (16)$$

where $\beta_b = \beta_s$. α_b is different from α_s and given by

$$\alpha_b = \frac{\Omega c_{\text{eq}}^0}{2} (D_1 - D_2) - \frac{\tilde{\Omega}\beta c_{\text{eq}}^0}{k_B T} \left(\frac{D_2}{x_2} + \frac{D_1}{x_1} \right). \quad (17)$$

When the difference in the diffusion coefficients is large, α_b is positive and the boundary is unstable against the fluctuation. By replacing ω with $\partial/\partial t$ and q with $\partial/\partial x$, the linear evolution equation of the fluctuation ζ is given by

$$\frac{\partial \zeta}{\partial t} = -\alpha_b \frac{\partial^2 \zeta}{\partial x^2} + \beta_b \frac{\partial^4 \zeta}{\partial x^4}. \quad (18)$$

By considering the symmetry of the system, the lowest-order nonlinear term is proportional to $(\partial\zeta/\partial x)^2$. The velocity in the y -direction of the inclined straight boundary is expanded as

$$V_b^0 \sqrt{1 + \left(\frac{\partial \zeta}{\partial x} \right)^2} = V_b^0 + \frac{V_b^0}{2} \left(\frac{\partial \zeta}{\partial x} \right)^2 + \dots \quad (19)$$

When we add the second term in eq. (19) to eq. (18), the nonlinear evolution equation is given by

$$\frac{\partial \zeta}{\partial t} = -\alpha_b \frac{\partial^2 \zeta}{\partial x^2} + \beta_b \frac{\partial^4 \zeta}{\partial x^4} + \frac{V_b^0}{2} \left(\frac{\partial \zeta}{\partial x} \right)^2. \quad (20)$$

The form of eq. (20) is the Kuramoto-Sivashinsky (KS) equation.^{21,22)} A solution of the KS equation exhibits spatio-temporal chaos.

When the distance between a step and a boundary is smaller than the surface diffusion lengths, we have to take account of the interaction of the fluctuations through the surface diffusion field. When the fluctuation of the phase boundaries is given by $\zeta_B(t)e^{iqx}$ and that of the steps is given by $\zeta_S(t)e^{iqx}$, the time evolutions of the amplitudes, $\zeta_S(t)$ and $\zeta_B(t)$, are given by

$$\begin{aligned} \frac{d\zeta_B}{dt} &= \frac{\Omega c_{\text{eq}}^0 D_1 \Lambda_{q1} [\cosh(\Lambda_{q1} l) \zeta_B + \zeta_S]}{x_1 \sinh(\Lambda_{q1} l)} \tanh \frac{l}{2x_1} \\ &\quad - \frac{\Omega c_{\text{eq}}^0 D_2 \Lambda_{q2} [\cosh(\Lambda_{q2} l) \zeta_B + \zeta_S]}{x_2 \sinh(\Lambda_{q2} l)} \tanh \frac{l}{2x_2}, \\ \frac{d\zeta_S}{dt} &= \frac{\Omega c_{\text{eq}}^0 D_2 \Lambda_{q2} [\cosh(\Lambda_{q2} l) \zeta_S + \zeta_B]}{x_2 \sinh(\Lambda_{q2} l)} \tanh \frac{l}{2x_2} \end{aligned} \quad (21)$$

$$- \frac{\Omega c_{\text{eq}}^0 D_1 \Lambda_{q1} [\cosh(\Lambda_{q1} l) \zeta_S + \zeta_B]}{x_1 \sinh(\Lambda_{q1} l)} \tanh \frac{l}{2x_1}. \quad (22)$$

In eqs. (21) and (22), we neglected the effect of the step stiffness for simplicity, and Λ_{q1} and Λ_{q2} are given by

$$\Lambda_{q1} = \frac{1}{x_1} \sqrt{1 + (qx_1)^2}, \quad (23)$$

$$\Lambda_{q2} = \frac{1}{x_2} \sqrt{1 + (qx_2)^2}. \quad (24)$$

When the distance l is shorter than the surface diffusion lengths and the wavelength of the fluctuation, the evolution equations, eqs. (21) and (22), are expressed as

$$\begin{aligned} \frac{1}{\Omega c_{\text{eq}}^0} \frac{d\zeta_B}{dt} &= - \frac{(D_1 - D_2)l^2}{4D_1 D_2} \Delta\zeta + \frac{(D_1 - D_2)}{4} \Delta\zeta q^2 \\ &\quad - \frac{l^2(D_2 - D_1)}{12\tau^2 D_1 D_2} \zeta_B q^2, \end{aligned} \quad (25)$$

$$\begin{aligned} \frac{1}{\Omega c_{\text{eq}}^0} \frac{d\zeta_S}{dt} &= - \frac{(D_2 - D_1)l^2}{4D_1 D_2} \Delta\zeta - \frac{(D_2 - D_1)}{4} \Delta\zeta q^2 \\ &\quad - \frac{l^2(D_1 - D_2)}{12\tau^2 D_1 D_2} \zeta_S q^2, \end{aligned} \quad (26)$$

where $\Delta\zeta = \zeta_S - \zeta_B$. The first terms in eqs. (25) and (26) express the changes of velocities given by eq. (7). If the steps and phase boundaries are fluctuated with the in-phase mode, i.e., $\zeta_B = \zeta_S$, the first and the second terms vanish. The amplitude of the fluctuation of the phase boundary increases and that of the step decreases.

4. Monte Carlo Simulation

From the linear stability analysis, step bunching does not occur. The step is stable, but the phase boundary is unstable against the wandering instability. To observe more detailed behavior than that obtained by the stability analysis, we carry out Monte Carlo simulations.

Near the structural transition temperature, the 7×7 and 1×1 structures coexist. The 7×7 structure is complicated, but to focus on the effect of the difference in the diffusion coefficients between the two structures, we use a simple model with a square lattice, in which the lattice constant $a = 1$. Except that the step is the non-Solid-on-Solid (non-SOS) type, the algorithm is similar to that in ref. 18. To model the difference in the diffusion coefficients, we vary the probability of adatom hopping. In the region with the large diffusion coefficient D_1 , an adatom at site (i, j) hops to site $(i \pm 1, j)$ with probability $D_1/4$. In the region with the small diffusion coefficient D_2 , D_1 is replaced by D_2 . Since the diffusion coefficient on the 1×1 structure is larger than that on the 7×7 structure, we set $D_1 = 1$ and $D_2 < D_1$ in our simulation. The hopping between the two regions occurs with the probability of hopping on the upper side. The boundary condition is helical in the y -direction and periodic in the x -direction. On average, the steps are parallel to the x -axis.

In our simulation, we distinguish between adatoms and solid atoms.^{23–26)} Active atoms comprise adatoms, the solid atoms at step edges, and those at structural boundaries. In a trial, we select an active atom. When the selected atom is an adatom, a diffusion trial or an evaporation trial is carried out. The probability of evaporation is given by $\Delta t/\tau$. The increment of time is $\Delta t = 1/4N_a$, where N_a is the number of adatoms.

In our model, two-dimensional nucleation is forbidden. Solidification occurs at the steps and the boundaries. After the diffusion trial, if the adatom attaches to a step edge or a structural boundary at the lower terrace, a solidification trial is carried out with the probability p_+ . When the selected atom is a solid atom, a melting trial is carried out with the probability p_- . The probabilities are given by²³⁾

$$p_{\pm} = \left[1 + \exp \left(\frac{\Delta E \mp \phi}{k_B T} \right) \right]^{-1}. \quad (27)$$

where ΔE_s is the increase of the step energy and ϕ is the decrease of the chemical potential by solidification. ΔE_s is given by $\Delta E_s = \epsilon \times$ (the increase of the step perimeter), where ϵ is the half of the step energy. In our simulation, we use $\epsilon/k_B T = 1.5$ and $\phi/k_B T = 3.0$.

We first study the formation of the pair consisting of a step and a structural boundary. Figure 2 shows the time evolution of step position and that of the boundary. The system size is 1024×1024 , $D_2 = 0.1$, and $\tau = 1024$. The long diffusion length is 32 and the short length is about 10. Initially, the step and boundary are straight, the position of the boundary is $y = 0$, and that of the step is $y = 512$. In our simulation, we use a helical boundary condition in the y -direction, but in Fig. 2 we show the evolution of absolute positions.

As expected from the linear stability analysis,¹⁶⁾ the receding step remains straight [Fig. 2(b)] and the receding boundary becomes unstable [Fig. 2(a)]. In the initial stage of the instability, the amplitude of fluctuation with the characteristic wavelength increases. The motion of protruding parts is chaotic in space and time. The pattern of the time evolution of the boundary is similar to the solution of the KS equation.^{21,22)}

Owing to the nonlinear term in the KS equation,^{21,22)} the boundary recedes faster than the step. The width of the region with the 7×7 structure becomes greater than that of the region with the 1×1 structure. When $0 < t < 5.2 \times 10^5$, the surface diffusion length in the 1×1 structure is shorter than the distance between the step and the structural boundary. Then, the interaction between them through the surface diffusion field becomes so weak that the step and boundary appear to be isolated.

Figure 3 shows the time evolution of the average positions of a step and a structural boundary. The dotted line represents the time evolution of the structural boundary and the solid line represents that of the step. In our simulation, we use a helical boundary condition in the y -direction. Thus, the position $y(x)$ is equal to $y(x) + L_y$. To clearly show the pairing of the step and boundary, we added L_y to the position of the boundary in Fig. 3. When we

Fig. 2. Time evolution of (a) a boundary and (b) a step with $0 < t < 5.2 \times 10^5$.

carry out a simulation with much longer interval, a collision between the step and structural boundary occurs. After the collision, the step and structural boundary coalesce and recede as a pair that does not separate again.

Fig. 3. Time evolution of positions of a step and a structural boundary. The dotted line represents the position of structural boundary and the solid line represents that of step.

Figure 4 shows the time evolution of the amplitude of the width of fluctuation $w(t)$, which is defined as

$$w(t) = \sqrt{\frac{1}{L_x} \left(\sum_{i=1}^{L_x} y(i, t) - \frac{1}{L_x} \sum_{i=1}^{L_x} y(i, t) \right)^2}, \quad (28)$$

where L_x is the system size in the x -direction and $y(i, t)$ is the y -coordinate of the step (structural boundary) at $x = i$. The width is averaged over 10 runs.

In the initial stage, the width of the structural boundary rapidly increases, but that of

the step remains small. Since the step recedes more slowly than the structural boundary, the distance between them decreases. With decreasing distance, the width of the structural boundary decreases and that of the step increases. When a collision between the step and structural boundary occurs, they coalesce and move as a pair. After the formation of the pair, the fluctuation of width of the pair increases with increasing time. In a later stage, the fluctuation of the width of is as large as that of the structural boundary in the initial stage ($t \approx 5 \times 10^5$).

Fig. 4. Time evolution of widths of step and structural boundary. Open circles represent the width of the step and open squares represent the width of the boundary.

Figure 5 shows the time evolution of position of a pair when $1.5 \times 10^6 < t < 4.0 \times 10^6$. Dotted lines and solid lines represent the positions of the boundary and step, respectively. The characteristic wavelength of wandering is longer than that of an isolated structural boundary, but the motion is similar to that given by a solution of KS equation.^{21,22)}

On a vicinal face, another type of instability, step bunching may occur. By carrying out Monte Carlo simulations with many steps, we study the possibility of step bunching occurring. Figure 6 is a snapshot of a vicinal face at $t = 2.0 \times 10^6$.

Number of steps N_s and that of boundaries N_b are $N_s = N_b = 4$. The system size is $L_x \times L_y = 1024 \times 512$. The diffusion coefficients are $D_1 = 1.0$ and $D_2 = 0.1$, and the lifetime of adatoms is $\tau = 256$. The long surface diffusion length is $x_1 = 16$ and short length is $x_2 \approx 5$. Initially, the steps and structural boundaries are equidistant. The average distance between them is 64, which is larger than the long surface diffusion length. In an early stage, pairs consisting of a step and structural boundary are formed. Owing to the large wandering of the pairs, the collision of pairs appears to occur.

From the snapshot (Fig. 6), we cannot establish whether the bunch size increases with increasing time or whether pairs collide. Next, we investigate the time evolution of the average positions of pairs (Fig. 7). Dotted lines represent the positions of structural boundaries and

Fig. 5. Time evolution of position of pair when $1.5 \times 10^6 < t < 4.0 \times 10^6$.

Fig. 6. Snapshot of a vicinal face at $t = 2.0 \times 10^6$. The number of boundaries N_b and that of steps N_s are $N_b = N_s = 4$. Initially, the steps and structural boundaries are equidistant.

solid lines represent those of steps. Initially, the steps and the structural boundaries are equidistant (Fig. 7(a)). The width of the pairs formed in an early stage fluctuates, but large bunches are not formed.

To form large bunches on the vicinal face, we may need to carry out the simulation for a longer period of times. Next, we set an isolated bunch in the initial stage and study the time evolution. Figure 7(b) represents the time evolution of an isolated bunch. Pairs consisting of a step and structural boundary are successively separated from the bunch. When we carry out a longer simulation, the bunch breaks to form an array of equidistant pairs.

In Figs. 6 and 7, the distance between each step and boundary on the vicinal face is longer than the surface diffusion lengths. We vary the long surface diffusion length and study how the motion changes. Figure 8 represents the time evolution of the vicinal face. The number of steps N_s and that of structural boundaries N_b are $N_s = N_b = 8$. The lifetime is $\tau = 4096$. The long surface diffusion length is 64, which is longer than the average distance between the step

Fig. 7. Time evolution of vicinal face. Number N_s of step and that N_b of boundary are $N_s = N_b = 4$. The simulation is started (a) with an equidistant array of steps and boundaries, and (b) with an isolated bunch.

and structural boundary, and the short length is about 20. Step bunching does not occur on a vicinal face (Fig. 8(a)), and each isolated bunch is unstable and breaks into pairs consisting of step and structural boundaries (Fig. 8(b)). With increasing surface diffusion length, the distance between the step and boundary in each pair increases, but the behaviors are similar to those in Fig. 7.

Fig. 8. Time evolution of one bunch. The number of steps N_s and that of boundaries N_b are $N_s = N_b = 8$. The simulation is started (a) with an array of equidistant steps and boundaries and (b) with an isolated bunch.

5. Summary and Discussion

In this paper, we studied the step instabilities on the Si(111) vicinal face near the $1 \times 1 \leftrightarrow 7 \times 7$ transition temperature during sublimation. To take account of the difference in the two structures, we considered the difference in their diffusion coefficients.

According to the linear analysis, the pairing of steps and phase boundaries does not occur. The step is stable and the phase boundary is unstable against step wandering. When we take account of the nonlinear effect, the motion of the boundary is given by a solution of the KS equation.^{21,22)} The motion of the boundary is expected to show a spatio-temporal chaos.

Owing to the nonlinearity of each solution of the KS equation,^{21,22)} the structural boundary recedes faster than the step, and their pairing occurs. The pair is also unstable against wandering. The wavelength of the fluctuation of the pair is longer than that of an isolated structural boundary, but the width of the fluctuation is as large as that of the structural boundary.

In an experiment,²⁷⁾ the surface diffusion length for the 1×1 structure at 900°C is estimated to be about $50\mu\text{m}$, and in a theoretical study,²⁸⁾ that on the surface with the 7×7 structure is calculated to be larger than a few μm . In an experiment,¹⁵⁾ both the widths of 1×1 structure and that of the 7×7 structure are smaller than the surface diffusion lengths. In our simulation, with increasing surface diffusion length, the difference in the widths of the two regions decreases. Thus, if we observe the formation of pairs consisting of a step and boundary during sublimation on the vicinal face, the difference in the width of the region with the 7×7 structure and that with the 1×1 structure is probably not large. Thus, we probably cannot observe the motion of bunches of tight pairs consisting of a step and boundary. However, Homma and co-workers^{29,30)} formed a large flat terrace with a width greater than $10\mu\text{m}$. On such a terrace, we can probably form a bunches of tight pairs consisting of a step and boundary. The wavelength of the fluctuation of the wandering of a pair is as long as the surface diffusion length. In this case, the time evolution of fluctuation of the pair may be observed.

In our model, we took account of the difference in the surface diffusion lengths and neglected the other differences. In the Si(111) surface, the number of adatoms used for a step to move is larger than that used for the structural boundary to move. The unit with the 7×7 structure is larger than that of the 1×1 structure. In our model, we neglected the differences between these structures and treated the structural boundary as the step. To quantitatively compare our results with experiments, we need to take account of the differences between the two structures in our model.

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