Step wandering on Si(111) vicinal face near the $1\times1\leftrightarrow7\times7$ transition temperature with drift of adatoms parallel to steps

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On a Si(111) surface, which is covered with the 1×1 structure at high temperature, the 7×7 structure appears when temperature is lower than the structural transition temperature (860 °C). On the vicinal face, the 7×7 structure spreads from the upper side of the step edge. The diffusion coefficient on the 1×1 structure is larger than that on the 7×7 structure. During growth, due to the difference in the diffusion coefficient, step wandering occurs and grooves perpendicular to the steps are formed. When the direct electric current is added parallel to the step, the grooves are tilted. In this paper, with taking account of the drift of adatoms caused by the direct current, we study the possibility of tilting of the grooves.

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A Si(111) surface is covered with the 1×1 structure at high temperature. When temperature is lower than the structural transition temperature ($\approx$860 °C), the 1×1 structure is reconstructed and the 7×7 structure appears. On the vicinal face near the transition temperature, the 7×7 structure is spread from the upper side of the step, and the two structures coexist in a terrace [1]. 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.

On the vicinal surface, there are two types of dynamical step instabilities, step wandering and step bunching. The step wandering is the instability for step deformation along the step, and the step bunching is that for the interstep distance. During growth [3], Hibino and co-workers observed the in-phase step wandering near the transition temperature. Due to the in-phase step wandering, grooves perpendicular to the steps appear. When direct electric current is parallel to steps, the grooves are tilted.

The step wandering on the vicinal face with the two structures has been studied [4,5]. When the difference in equilibrium adatom density between the two structures is neglected and that in the diffusion coefficient is taken into account, the step wandering occurs and the grooves are formed during growth. However, the effect of the drift, which is considered to be caused by the current, on tilting of grooves has not been studied.

In this paper, bearing the growing Si(111) vicinal face with the two structures in mind, we study the possibility of tilting of grooves by the drift. We take account of the difference in diffusion coefficient, and use the model of Kato *et al.* [5], in which the ratio of the widths between two structures can be changed.

We consider a vicinal face, where the x direction is parallel to the step and the y direction is toward the step-down direction (Fig. 1). When we neglect the evaporation of adatoms, the diffusion equation, which the adatom density $c(\boldsymbol{r},t)$ obeys, is given by

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

where f is the impingement of adatoms and $\boldsymbol{j}(\boldsymbol{r},t)$ is the adatom current on the surface. When the drift of adatoms is parallel to the x axis, the adatom current is given by

$$\boldsymbol{j}(\boldsymbol{r},t) = -D_s(\boldsymbol{r})\left(\nabla c(\boldsymbol{r},t) - \frac{F_d c(\boldsymbol{r},t)}{k_B T}\hat{e}_x\right), \tag{2}$$

where $D_s(\boldsymbol{r})$ is the local diffusion coefficient, and F_d is the force to cause the drift. $D_s(\boldsymbol{r})=D_1$ on the 1×1 structure on the lower side of a step and $D_s(\boldsymbol{r})=D_2$ on the 7×7 structure on the upper side of a step.

From experiment [2], the diffusion coefficient on the 1×1 structure is larger than that on the 7×7 structure. Then, we assume D_1 is larger than D_2.

The structural boundary advances with absorbing adatoms and recedes with releasing adatoms [6], which is similar to the step. When the structural boundary moves, the number of adatoms for the structural boundary to use is much fewer than that for the step [7]. However, following Kato *et al.* [5], we neglect the difference in properties between step and structural boundary, and treat a structural boundary as a step. At steps and structural boundaries, we assume that the adatom densities are in equilibrium: $c|_{s(b)}=c_{eq}^{s(b)}$, where s(b) indicates the step (the structural boundary) position. The approximation implies an infinite kinetic coefficient. We should take account of the effect of kinetic coefficient, but for simplicity, we use the assumption in this paper. The equilibrium adatom density c_{eq}^{s} at the step and that c_{eq}^{b} at the structural boundary are given by $c_{eq}^{s(b)}=c_{eq}^{0}(1+\Omega\tilde{\beta}\kappa^{s(b)}/k_BT)$, where c_{eq}^{0}

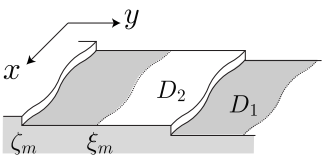

FIG. 1. A Si(111) vicinal face near $1\times1\leftrightarrow7\times7$ structural transition temperature.

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is the equilibrium adatom density at the isolated step, Ω is atomic area, $\tilde{\beta}$ is step stiffness, and $\kappa^{s(b)}$ are the curvatures.

By solving the diffusion equation, Eq. (1), with boundary conditions in the quasistatic approximation ($\partial c/\partial t=0$), the velocity V_s of step and that V_b of structural boundary are given by $V_{s(b)}=\Omega(\boldsymbol{j}|_{s(b)-}-\boldsymbol{j}|_{s(b)+})\cdot\boldsymbol{n}_{s(b)}$, where +(−) indicate the lower (upper) side of the step and structural boundary, and $\boldsymbol{n}_{s(b)}$ is the normal vector of the step (structural boundary) toward the step-down direction.

We carry out linear stability analysis for the wandering instability. We assume that steps and structural boundaries are straight. When they are equidistant with distance l, the mth position $\zeta_m^0(t)$ of step and $\xi_m^0(t)$ of structural boundary are given by $\zeta_m^0(t)\equiv V_s^0 t+2ml$, $\xi_m^0(t)\equiv V_b^0 t+(2m+1)l$. The adatom density $c_1^0(y)$ in the region with large diffusion coefficient D_1 and $c_2^0(y)$ in the region with small diffusion coefficient D_2 are given by

$$c_1^0(y)=-\frac{f}{2D_1}(y-\zeta_m^0)^2+\frac{fl}{2D_1}(y-\zeta_m^0)+c_{eq}^0, \tag{3}$$

$$c_2^0(y)=-\frac{f}{2D_2}(y-\xi_m^0)^2-\frac{fl}{2D_2}(y-\xi_m^0)+c_{eq}^0, \tag{4}$$

where $c_1^0(y)$ is defined in $\zeta_m^0\le y\le\xi_m^0$ and $c_2^0(y)$ is defined in $\xi_m^0\le y\le\zeta_{m+1}^0$. The velocities, V_s and V_b are given by $V_s^0=V_b^0=fl$.

We give sinusoidal perturbations with the wave number k to the steps and the structural boundaries. When the perturbation to the mth step is $\delta\zeta_m(t)e^{ikx}$ and that to the mth structural boundary is $\delta\xi_m(t)e^{ikx}$, due to the fluctuations, the adatom density $c_1(\boldsymbol{r},t)$ is modified and given by $c_1(\boldsymbol{r},t)=c_1^0(y)+\delta c_1(\boldsymbol{r},t)e^{ikx}$. The boundary conditions are given by

$$\delta c_1|_{\zeta_m^0}+\left.\frac{dc_1^0}{dy}\right|_{\zeta_m^0}\delta\zeta_m(t)=k^2\Gamma\,\delta\zeta_m(t), \tag{5}$$

$$\delta c_1|_{\xi_m^0}+\left.\frac{dc_1^0}{dy}\right|_{\xi_m^0}\delta\xi_m(t)=k^2\Gamma\,\delta\xi_m(t), \tag{6}$$

where $\Gamma=\Omega c_{eq}^0\tilde{\beta}/k_BT$. By considering the similar equations for $c_2(\boldsymbol{r},t)$, we obtain the derivative equations for $\zeta_m(t)$ and $\xi_m(t)$. When $\xi_m(t)$ and $\zeta_m(t)$ are expressed as $\xi_m(t)=\xi(t)e^{i(2m+1)\phi l}$ and $\zeta_m(t)=\zeta(t)e^{i2m\phi l}$, the derivative equation for $\zeta(t)$ is given by

$$\frac{d\zeta}{dt}=\frac{ifl\Lambda_k\sin\phi l}{\sinh\Lambda_k l}\xi+i\frac{\Delta D_s\Gamma\Lambda_k k^2}{\sinh\Lambda_k l}\xi\sin\phi l+\frac{2D_s\Gamma\Lambda_k k^2}{\sinh\Lambda_k l}(\xi\cos\phi l-\zeta\cosh\Lambda_k l), \tag{7}$$

where $\Delta D_s=D_1-D_2$, $D_s=(D_1+D_2)/2$, and ϕ is the shift of phase between the step and the structural boundary. Λ_k is given by $\Lambda_k=\sqrt{k^2+ikf_d}$ with $f_d=F_d/k_BT$. We obtain the derivative equation for $\xi(t)$ by replacing $\xi(t)$ to $\zeta(t)$ and D_1 to D_2.

From the derivative equations, the amplification rates of the fluctuations are given by

$$\omega_\pm=-\frac{2\Gamma k^2D_s\Lambda_k}{\tanh\Lambda_k l}\pm\frac{\Lambda_k}{\sinh\Lambda_k l}\sqrt{(\Gamma k^2\Delta D_s\sin\phi l)^2+h(k,\phi)}, \tag{8}$$

where $h(k,\phi)$ is expressed as $h(k,\phi)=(2\Gamma k^2D_s\cos\phi l+ifl\sin\phi l)^2$. The relation between ζ and ξ is given by $\zeta=\alpha\xi$ when the amplification rate is $\omega=\omega_+$, and $\zeta=-\alpha\xi$ when the amplification rate is $\omega=\omega_-$, where α is given by

$$\alpha=\sqrt{\frac{ifl\sin\phi l+\Gamma k^2(2D_s\cos\phi l+i\Delta D_s\sin\phi l)}{ifl\sin\phi l+\Gamma k^2(2D_s\cos\phi l-i\Delta D_s\sin\phi l)}}. \tag{9}$$

When the impingement rate is small, the amplification rates are expressed as

$$\omega_\pm=\frac{\pm ifD_s\Lambda_k l\sin\phi l\cos\phi l}{\sinh\Lambda_k l\sqrt{D_s^2-D_1D_2\sin^2\phi l}}-2D_s\frac{\Gamma k^2\Lambda_k}{\sinh\Lambda_k l}\left(\cosh\Lambda_k l\mp1\pm\frac{4D_1D_2\sin^2\phi l}{2D_s^2}\right). \tag{10}$$

If the wavelength of the fluctuation is long and the shift of the phase is small, $\omega_\pm$ are approximated as

$$\omega_+=i(f\phi-\Gamma D_sf_dk^3)l+\frac{f_df\phi l^3}{3!}k-\Gamma D_sl\left(k^2+\frac{D_1D_2\phi^2}{D_s^2}\right)k^2, \tag{11}$$

$$\omega_-=-i\left(f\phi+\frac{\Gamma D_sf_d}{3}k^3\right)l-\left(\frac{f_df\phi l^3}{3!}k+\frac{4\Gamma D_s}{l}k^2\right). \tag{12}$$

The real part of $\omega_\pm$ is the growth rate of the amplitude of fluctuation. When the real part is positive, the wandering occurs. If the drift of adatoms is present and the phase shift, ϕ is finite, the impingement causes the step wandering. Since the effect of the step stiffness in ω_- is larger than that in ω_+, the amplitude of the fluctuation with ω_+ grows faster than that with ω_-.

The step wandering with ω_+ occurs when $f_d\phi$ is positive. If ϕ is so small that ϕ^2 is neglected, the wavelength of the most unstable mode, λ_{max} is given by

$$\lambda_{max}=2\pi\left(\frac{12\Gamma(D_1+D_2)}{f_df\phi l^2}\right)^{1/3}. \tag{13}$$

The growth rate of the amplitude for the mode, Re ω_{+max} is given by

$$\mathrm{Re}\;\omega_{+max}=\frac{1}{8}\left(\frac{f_d^4f^4\phi^4l^{11}}{12\Gamma(D_1+D_2)}\right)^{1/3}. \tag{14}$$

To study the behavior of unstable step in detail, we carry out Monte Carlo simulation. We consider a square lattice with the lattice constant $a=1$. The steps and the structural boundaries are parallel to the x direction on average and the step-down direction is in the y direction. The boundary condition is periodic in the x direction and helical in the y direction.

To forbid a step to overlap with a structural boundary, we take account of the short-range repulsion between a step and a structural boundary, but neglect the long-range repulsion.

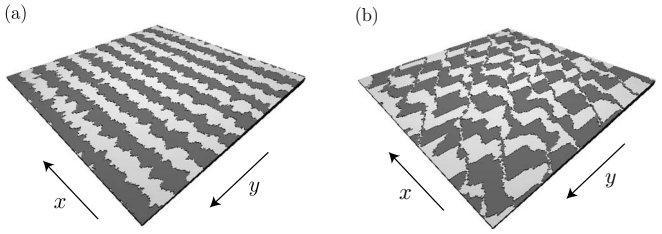

FIG. 2. Snapshots without the difference in the diffusion coefficient. The diffusion coefficients are $D_1=D_2=1$: (a) without drift and (b) with drift.

The steps and the structural boundaries obey the solid-on-solid condition: The positions of them are given by single-valued functions of x.

In our model, solid atoms at steps, those at structural boundaries and adatoms are active. In a trial, we randomly choose an active atom. If an adatom is chosen, hopping trial is carried out. When the adatom is on the region with fast diffusion, the adatom on a site (i,j) hops to $(i,j\pm1)$ with the hopping probability $D_1/4$ and hops to $(i\pm1,j)$ with the probability $D_1(1\pm F_d/k_BT)/4$, where F_d is the force to cause the drift of adatoms. When the adatom is on the region with slow diffusion, D_1 is replaced to D_2. The hopping between the two regions is carried out with the hopping probability on the upper side region. Except for the hopping probability, the algorithm is similar to other studies [8–10]. The time increase Δt in a hopping trial is $\Delta t=1/(4N_a)$, where N_a is the number of adatoms. If the adatom attaches to a step (structural boundary) from a 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 p_- of melting are given by

$$p_\pm = \left[1+\exp\left(\frac{\Delta E_s \pm \phi_c}{k_BT}\right)\right]^{-1}, \tag{15}$$

where ΔE_s is the increase of the step energy and ϕ_c 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 one-half of the step energy. After some diffusion trial, the impingement of adatoms is tried if the adatom density is lower than that in equilibrium.

Figure 2 represent snapshots of step wandering without the difference in the diffusion coefficients during growth. The diffusion coefficients are $D_1=D_2=1$. Parameters are $\epsilon/k_BT=0.8$, $\phi/k_BT=1.5$, and the impingement rate $f=1.0\times10^{-3}$. The system size is $L_x\times L_y=512\times512$. The number of steps and that of structural boundary is 8. The diffusion coefficient is D_1 in the dark region and D_2 in the light region. In Fig. 2(a), the drift is absent. The step wandering does not occur, and the steps and the structural boundaries are straight with small fluctuation. In Fig. 2(b), the drift is in the x direction $(F_da/2k_BT=0.3)$. The step wandering occurs, and, with increasing y coordinate, the wandering pattern is shifted to the opposite of the drift. Then, $f_d\phi$ is positive, which agrees with the linear stability analysis.

Figure 3 represents a snapshot with the difference in the diffusion coefficient during growth. The diffusion coefficients are $D_1=1$ and $D_2=0.3$. The other parameters are the same as those in Fig. 2. With the drift parallel to the x direction $(F_da/2k_BT=0.3)$, the step wandering occurs. The amplitude of fluctuation of the structural boundary is so small that the wandering of the structural boundaries does not seem to occur, which is different from Fig. 2(b).

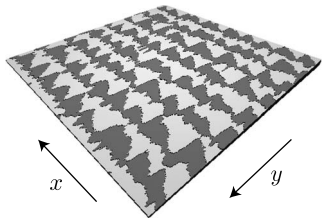

FIG. 3. Snapshots with the difference in the diffusion coefficient. The diffusion coefficients are $D_1=1$ and $D_2=0.3$.

From the linear stability analysis, the ratio of the amplitude of the fluctuation of step to that of structural boundary is determined by parameter α. When D_1 is equal to D_2, irrespective of ϕ, the amplitude of α is $|\alpha|=1$. When D_1 is larger than D_2, $|\alpha|$ increases with increasing ϕ, and $|\zeta|$ becomes larger than $|\xi|$. Thus, the results of simulation are consistent with the linear analysis.

In this paper, bearing Si(111) vicinal face consisting of 1×1 structure and 7×7 structure in mind, we studied the possibility of the drift-induced step wandering during growth. As the difference in the two structures, we took account of the difference in the diffusion coefficient: The diffusion coefficient on the 1×1 structure is faster than that on the 7×7 structure. The structural boundary advances with absorbing adatoms and recedes with releasing atoms, which is similar to the step. Thus, in our study, we regard a structural boundary as a step.

From the linear stability analysis, the step wandering occurs when the drift is parallel to the steps. With increasing the numbering of steps, the wandering pattern is shifted opposite to the drift. The amplitude of the fluctuation of structural boundary is as large as that of steps without the difference in the diffusion coefficient, but smaller than that of steps with the difference, which agree with Monte Carlo simulation.

In the experiment [3], Hibino and co-workers observed the step wandering on the Si(111) vicinal face near the structural transition temperature. The wandering is caused by the impingement. On the Si(111) vicinal face in other temperature regimes [12], the wandering is caused by the drift of adatoms. Thus, the mechanism of wandering [3] is different of that in other temperatures. When the current is parallel to the step, the wandering with the shift of phase ϕ occurs. Since the current and the drift of adatoms are in the same direction, the product of the drift velocity and the shift of phase, $f_d\phi$ is positive, which agrees with our results. However, in our model, the step wandering does not occur when the drift is absent, which disagrees with the experiment [3]. The disagreement is probably caused because we assumed that the kinetic coefficients are infinite.

If we neglected the difference in the diffusion coefficient, our model and the model by Liu and co-workers [11] are the

same. The relation of the phase of wandering pattern and the drift direction is the same as that in Ref. [11]. However, in their model, the wandering occurs without the impingement of adatoms, which does not agree with our model. The disagreement is also caused by the infinite kinetic coefficient. In our linear analysis, the step wandering occurs without the difference in the diffusion coefficient. However, as shown in Fig. 2(b) and Fig. 3, the wandering pattern is influenced by the difference in the diffusion coefficient. Thus, the difference is important in the instability.

Zhao and co-workers [13] also studied the step instability by the model with two regions. In their model, the diffusion coefficient in a small region around step is different from that in a large terrace, and the effect of difference in the diffusion coefficient is reduced to a finite kinetic coefficient. In our model, the diffusion coefficient in the lower side of step is different from that in the upper side. Our model is different from the model by Zhao and co-workers. Thus, we cannot simply compare their model with our model. We will study this with more detail in the future.

In the Si(111) vicinal face, the number of adatoms for the structural boundary to use to advance is fewer than that at step, which is probably expressed as the small kinetic coefficient in the step flow model. To compare the analysis with the experiment in detail, we need to take account of the effect of the kinetic coefficient.

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