Electric-current-induced step bunching on Si(111)

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We experimentally investigated step bunching induced by direct current on vicinal Si(111)''1×1'' surfaces using scanning electron microscopy and atomic force microscopy. The scaling relation between the average step spacing l_b and the number of steps N in a bunch, $l_b \sim N^{-\alpha}$, was determined for four step-bunching temperature regimes above the 7×7-''1×1'' transition temperature. The step-bunching rate and scaling exponent differ between neighboring step-bunching regimes. The exponent α is 0.7 for the two regimes where the step-down current induces step bunching (860–960 and 1210–1300 °C), and 0.6 for the two regimes where the step-up current induces step bunching (1060–1190 and >1320 °C). The number of single steps on terraces also differs in each of the four temperature regimes. For temperatures higher than 1280 °C, the prefactor of the scaling relation increases, indicating an increase in step-step repulsion. The scaling exponents obtained agree reasonably well with those predicted by theoretical models. However, they give unrealistic values for the effective charges of adatoms for step-up-current-induced step bunching when the ''transparent'' step model is used.

I. INTRODUCTION

A decade has passed since the direct current (dc) effect on atomic step bunching on Si(111) was found by Latishev *et al.*[1] Step bunching is an instability of the regular distribution of atomic steps on a vicinal surface under an external field, and an attractive topic theoretically because there are at least four transitions where the direction of step-bunching-inducing current reverses. These transitions occur at the 7×7-''1×1'' transition temperature of 860 °C, around a gap between 1000 and 1060 °C, and at 1200 and 1300 °C (these temperatures vary at most by 50 °C in the literature[1–3]). Specifically, a step-down current induces step bunching in the temperature ranges of $860 < T < 960$ °C and $1200 < T < 1300$ °C, while a step-up current causes step bunching in the ranges of $1060 < T < 1200$ °C and $T > 1320$ °C. There is further complication during the 7×7-''1×1'' transition in that the step-bunching-inducing-current direction changes twice, depending on the coverage of 7×7 domains.[4] For the step-bunching mechanism, Stoyanov proposed a model of adatom electromigration[5] based on a generalized Barton-Cabrera-Frank (BCF) theory.[6] In this model, step bunching occurs when the adatom electromigration is in the step-down direction. Since the adatoms on Si(111) are thought to be positively charged,[7] this model describes the step bunching under the step-down current. On the other hand, the step-up current stabilizes the regular arrangement of atomic steps in the framework of the BCF-based model. Misbah, Pierre-Louis, and Pimpinelli suggested that advacancys, which move in the opposite direction to adatoms, can cause the inversion of the step-bunching field direction at high temperatures.[8] Kandel and Kaxiras argued that the sign of effective charge changes depending on temperature.[9]

Recently, Stoyanov proposed a different mechanism of step bunching under the step-up current.[10] In the framework of BCF theory, atomic steps are adatom diffusion boundaries, so the motion of a step is determined by the terrace in front of it and the one behind it. In Stoyanov's new model, on the contrary, adatoms can cross steps, so the steps are said to be transparent (or permeable). In this situation, the adatom concentration distribution is determined by the local step density and the effect of electromigration. This model shows that step bunching takes place for the step-up electromigration of adatoms. Thus, it was subsequently proposed that the transition from step-down-current-induced to step-up-current-induced bunching is due to changes in atomic step properties, such as the density of kinks in a step changing from high to low. This model explains the inversion of step-bunching-inducing-current direction under growth circumstances in the 1060–1200 °C regime.[11] Suga *et al.*, on the other hand, proposed another mechanism of current direction inversion quite recently.[12] They took into account external-force dependence in the mass transport of adatoms, and showed that the step-down force induces step bunching in a capture-limited case, while the step-up direction force induces it in a diffusion-limited case. Their model suggests that the change in adatom transport mechanism with temperature causes the inversion of step-bunching-inducing-current direction. This model reproduces step wandering in the regular distribution of steps, which was found recently under step-up current in the 1060–1200 °C regime,[13] assuming diffusion-limited kinetics.

Various step-bunching mechanisms have been proposed, as we have seen above. However, they are still controversial, and no single model explains all of the inversions of step-bunching-inducing-current direction. It should be mentioned that Liu and Weeks discussed the effects of step permeability and capture-limited/diffusion-limited step dynamics for step bunching near 900 °C, and showed no transitions caused by these effects.[14] Therefore, it is essential that existing models be tested by quantitatively comparing them with experi-

ments. Stoyanov and Tonchev predicted a scaling relation between the minimum terrace size $l_{\min}$ and number of steps N in a bunch, $l_{\min} \sim N^{-\alpha}(A/F)^q$, where A is the magnitude of step-step repulsion and F is the force for electromigration of adatoms.[15] The scaling exponents α and q depend on the power n in the step-spacing dependence of the step-step repulsion ($U=A/l^n$) and the bunching mechanism (e.g., BCF-type steps or transparent steps). Fujita, Ichikawa, and Stoyanov reported scaling exponents at 1145 °C (under the step-up current) and 1250 °C (under the step-down current).[16] Their results are consistent with the transparent step model with $n=2$ at 1145 °C and a BCF-type model with $n=2$ at 1250 °C.

The aim of this paper is to provide systematic experimental data for step bunching in a wide temperature range, so that the data can be compared to theoretical models. We measured the step-bunch shapes for temperatures higher than the 7×7-''1×1'' transition temperature and determined the scaling relations $l_{\min} \sim N^{-\alpha}$ for each bunching temperature regime. The scaling exponents were compared with theoretical scaling exponents of the BCF and transparent-step models.

II. EXPERIMENTAL PROCEDURE

We used an ultrahigh vacuum scanning electron microscope[17] (UHV-SEM) to resistively heat specimens and observe step-bunch evolution. The vicinal Si(111) substrates mainly used were a boron-doped (~5 Ω cm) wafer 0.15° miscut toward the $\langle \overline{1}\,12 \rangle$ direction and a phosphorus-doped (~3 Ω cm) wafer 1° miscut toward the $\langle 11\overline{2} \rangle$ direction. A boron-doped (~10 Ω cm) wafer 1° miscut toward the $\langle 1\overline{1}0 \rangle$ direction was used for comparison. Specimens $20\times5\times0.4\,\mathrm{mm}^3$ were cut from these wafers. The long side of the specimen was parallel to the miscut orientation. After oxidation using H_2SO_4:H_2O_2(4:1) solution the specimens were introduced into the UHV-SEM and resistively heated using direct current. The temperature was measured using an infrared pyrometer, which was calibrated using a disappearance filament pyrometer taking into consideration the temperature dependence of emissivity.[18] We estimate the accuracy of temperature measurements to be ±20 °C around 1200 °C. These temperatures were about 10 °C higher than in our previous paper[2] because of the difference in the calibration procedures. It is reasonable to note that there are some differences among the reported transition temperatures of the step-bunching current inversion as well as the 7×7-''1×1'' transition temperature. Our current inversion temperature of 1200 °C from step-up to step-down current corresponds to the 1250 °C inversion in Refs. 1 and 11. In our measurements, the 7×7-''1×1'' transition temperature on Si(111) was 860 °C, while Ino reported that the transition occurred at 830 °C,[19] which has been cited in many papers. Phaneuf and Williams also reported an 860 °C transition temperature.[20]

Temperatures examined ranged from 910 to 1360 °C. To obtain these temperatures, about 7 V was applied across the 17 mm gap of the specimen with current of 3–13 A. Each specimen was used repeatedly to obtain several temperature data. Before each step-bunching experiment, steps were debunched at 1230 °C by passing the specimen through the step-up direction current. Care was taken to eliminate any bunching morphology formed in the preceding experiment. To observe evolution of step bunches at each temperature, the specimen was repeatedly heated for a certain time interval and cooled to about 350 °C for SEM observation. The rate of cooling from above 1200 to 600 °C was about 150 °C/s. During heating, the specimen chamber pressure was kept at less than 5×10^{-7} Pa.

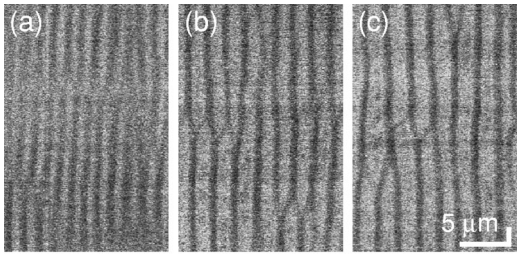

FIG. 1. SEM images of step-bunch evolution on vicinal Si(111) 1° miscut toward the $\langle 11\overline{2} \rangle$ direction at 1256 °C. Darker regions are step bunches. Heating times were (a) 30, (b) 60, and (c) 90 s.

The SEM was operated with a 25 keV electron beam at a 70° incident angle. Examples of SEM images of step bunches are shown in Fig. 1 for 1256 °C in the step-down current direction. Average values of apparent terrace with L_t' and bunch width L_b' were derived from SEM images at several positions. These apparent widths are the lengths projected on the initial vicinal surface. The actual terrace width L_t, bunch width L_b, and bunch height H are given by $L_t = L_t'/\cos\theta$, $L_b = (L_t' + L_b')\cos\theta - L_t$, and $H = (L_t' + L_b')\sin\theta$, where θ is the miscut angle of the vicinal surface. Then the number of steps in a bunch N can be obtained as $N = H/h_0$ by using the height h_0 of a single step on Si(111), and the average step spacing in a bunch is $l_b = L_b/N$. Since the slope of a step bunch can be regarded as almost constant, we used l_b instead of $l_{\min}$. After removing the specimens from the vacuum, atomic force microscopy (AFM) was employed to evaluate step-bunch shapes directly in air.

III. RESULTS

In a step-bunching condition, the bunch-size evolution occurs as a result of interaction between step bunches as seen in Fig. 1. On average, the number of steps in a step bunch increases with heating time. The time dependence of the average step number in a bunch is shown in Fig. 2 for various temperatures. The step number increased roughly in proportion to $t^{0.5}$. This result corresponds to the $t^{0.5}$ dependence of terrace width reported by Yang, Fu, and Williams.[3] The figure also indicates a large temperature dependence of the bunching rate. Although the bunching rate was not constant, a mean bunching rate in the initial stage of bunching would be helpful to illustrate an outline of the temperature dependence of step-bunching phenomena. Thus, average bunching rates were derived using linear fits of the 1° data and are shown in Fig. 3. Now the four bunching regimes above the 7×7-''1×1'' transition temperature (860 °C) are clearly seen. The bunching rate changed by more than two orders of magnitude over the four regimes, from less than 10^{-2} to 1 steps/s. A striking difference in the bunching rate is that around the 1200 °C transition. In spite of a small temperature

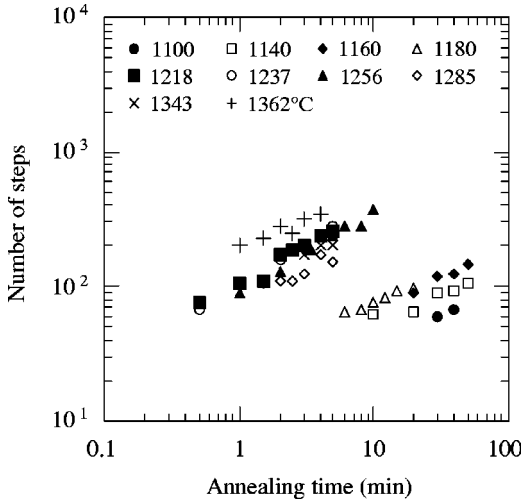

FIG. 2. Time dependence of average number of steps in a step bunch on vicinal Si(111) 1° miscut toward the $\langle 11\bar{2}\rangle$ direction at various temperatures.

gap, the bunching rate jumps by a factor of 20 from 1180 to 1210 °C. The bunching-rate difference around the 1300 °C transition is small. Another notable thing is that no bunching takes place between 960 and 1060 °C. The widths of the other two gaps where no bunching occurs were less than 30 °C. We hereafter refer to these bunching temperature regimes as regime 1 (step down, $860<T<960$ °C), regime 2 (step up, $1060<T<1200$ °C), regime 3 (step down, $1200<T<1300$ °C), and regime 4 (step up, $T>1320$ °C).

The size scaling relationship between the average step distance l_b and the number of steps in the bunch N is shown in Fig. 4(a) for various temperatures. The SEM data from regimes 2–4 are plotted altogether. To obtain wide N values, the data for both 0.15° and 1° miscut substrates were used. Except for temperatures higher than 1280 °C, the data were scaled in a narrow region. That is, the differences in scaling exponents and prefactors were small for different tempera-

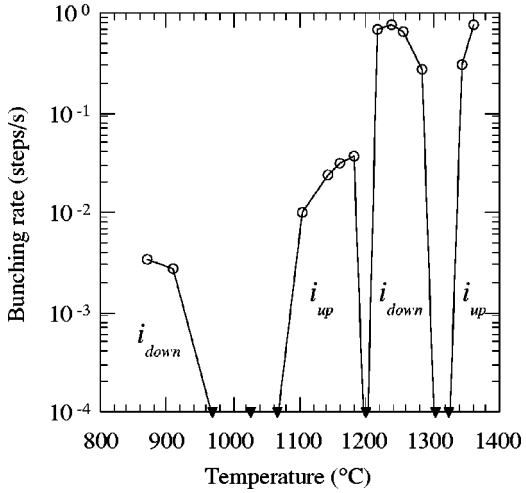

FIG. 3. Temperature dependence of step-bunching rate on vicinal Si(111) 1° miscut toward the $\langle 11\bar{2}\rangle$ direction. The bunching rate was determined as an average rate in the initial stage of step bunching. i_{down} and i_{up} denote the step-down-current-induced and step-up-current-induced step bunching.

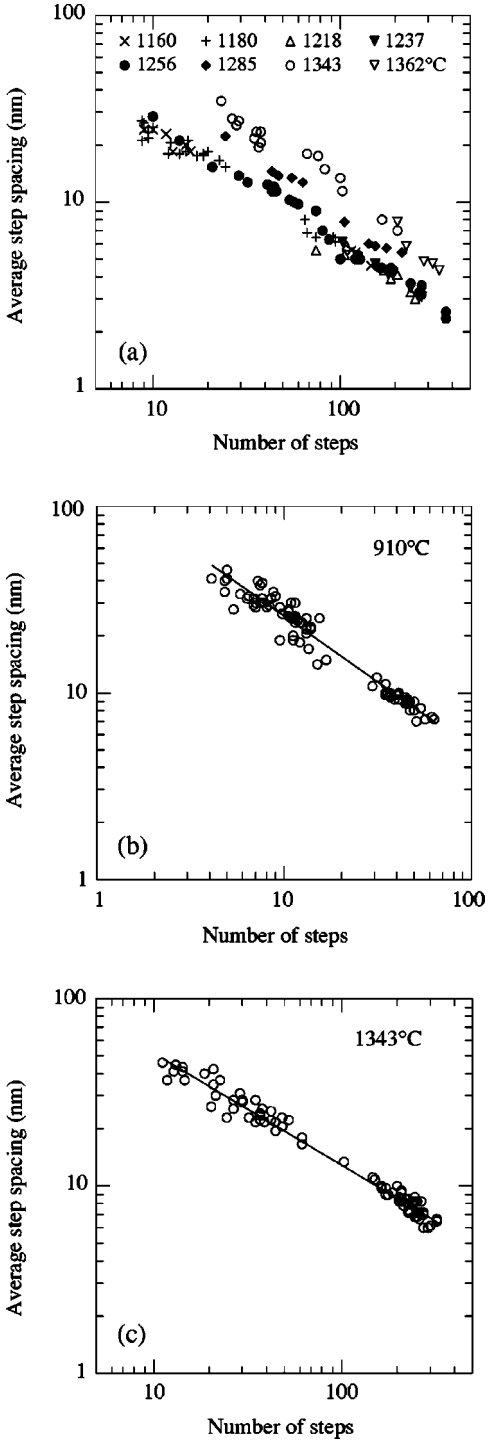

FIG. 4. Average step spacing in a step bunch as a function of the number of steps in a bunch. The data were obtained using vicinal Si(111) surfaces 0.15° miscut toward the $\langle \bar{1}\,\bar{1}2\rangle$ direction and 1° miscut toward the $\langle 11\bar{2}\rangle$ direction. (a) SEM data for regimes 2–4. (b) AFM data for regime 1 (910 °C). (c) AFM data for regime 4 (1343 °C).

ture regimes. It should be noted that the scaling relation did not depend on the step orientation. Figure 4(a) includes the data for $\langle \bar{1}\,\bar{1}2\rangle$ steps of the 0.15° miscut surface and $\langle 11\bar{2}\rangle$ steps of the 1° miscut surface. We also examined $\langle 1\bar{1}0\rangle$-oriented steps and confirmed that these steps showed the same l_b vs N relationship within the experimental error.

TABLE I. Experimental size scaling parameters for the four temperature regimes and F/A and z_{eff} calculated using the BCF-type or transparent-step model. The A values are from Ref. 25 for the Si(111) ''1×1'' surface without short-range order.

Regime	T (°C)	Prefactor	Exponent	F/A (nm^{-2})	A (eV nm)	F ($\mathrm{eV\,nm}^{-1}$)	z_{eff} ($\lvert e\rvert$)
1	910 (AFM)	128	0.70	6.4×10^{-7}[a]	0.06	4.0×10^{-8}	0.1
2	1160 (SEM)	98	0.61	1.6×10^{-5}[b]	0.17	2.7×10^{-6}	7
	1180 (SEM)	95	0.59	1.9×10^{-5}[b]	0.19	3.6×10^{-6}	9
3	1237 (SEM)	163	0.70	3.1×10^{-7}[a]	0.25	7.8×10^{-8}	0.2
	1256 (SEM)	133	0.66	5.7×10^{-7}[a]	0.30	1.7×10^{-7}	0.4
	1285 (SEM)	220	0.71	1.3×10^{-7}[a]	0.34	4.3×10^{-8}	0.1
4	1343 (SEM)	232	0.64	2.1×10^{-7}[b]	0.56	1.2×10^{-7}	0.3
	1343 (AFM)	202	0.59	4.2×10^{-7}[b]	0.56	2.4×10^{-7}	0.6

[a]BCF-type model (Ref. 15).
[b]Transparent-step model (Ref. 10).

The independence of step character is peculiar to dc-induced step-bunching phenomena. Transition temperatures are the same for different orientations of steps.[4]

In Fig. 4(a), each temperature data set was obtained from SEM images at various heating times. However, in regime 1 it was difficult to obtain a large number of data points because the bunching rate was so low. Accordingly, we used AFM images of step bunches at fixed heating time (4 h for the 0.15° miscut surface and 2 h for the 1° miscut surface) and measured l_b and N for different sizes of bunches. Figure 4(b) is the plot for 910 °C using AFM data. Although the scatter of 0.15° data (smaller-N data) is large, they can be regarded as having the same N dependence as the 1° data (large-N data). The data at 910 °C also lie within the region shown in Fig. 4(a). AFM data are shown in Fig. 4(c) for regime 4, where only a small number of SEM data were measured. For other regimes, the SEM-based values were confirmed to be consistent with AFM-based values.

Although most of the data were scaled in the narrow region, there were sizable differences in the scaling exponents from different temperature regimes. The exponents and prefactors were derived from data set with a wide range of N, and are listed in Table I. The exponents were 0.70 ± 0.03 in regime 1, 0.60 ± 0.03 in regime 2, 0.69 ± 0.03 in regime 3, and 0.64 ± 0.05 (SEM) or 0.59 ± 0.03 (AFM) in regime 4. The error on the SEM result in regime 4 was larger than in other regimes, so we adopted the AFM result in this regime. The exponent was 0.59–0.60 for the two regimes where step bunching was induced by the step-up current, and 0.69–0.70 for the two regimes where the step-down current induced step bunching. These exponents in regimes 2 and 3 are in agreement with the values reported by Fujita, Ichikawa, and Stoyanov (0.60 ± 0.04 at 1145 °C and 0.68 ± 0.03 at 1250 °C).[16] Another important result is the substantial temperature dependence of the scaling relationship at higher temperatures. This change was evident for the 1285 °C data in regime 3 and became larger in regime 4. This was due to the change in the prefactor, but the exponent remained almost the same within the experimental error. Since it was difficult to obtain reliable prefacters from all data sets, the average step spacing at the step number of 100 was taken as a measure of the change. The step spacing at $N=100$ is shown in Fig. 5. The spacing gradually increased with an apparent ''activation'' energy of 0.7 eV. This increase in step spacing implies that there was a change in the magnitude of step-step interaction. This increase may be attributed to entropic repulsion. Thus, the apparent ''activation'' energy does not mean the presence of an actual activation barrier.

It is worth noting the differences observed in the step-bunch shape and the number of crossing steps on a terrace region between step bunches. Figure 6 shows AFM images of step bunches for the four temperature regimes. It is obvious that the step bunch in regime 4 is less steep compared to the other three regimes, even though the number of steps in a bunch in Fig. 6(d) is much larger than in the others. This is due to a larger l_b value, as mentioned above. Another interesting and important finding is that the number of crossing steps on a terrace region is different for the four regimes. In regime 1, most terraces had no crossing steps. The lowest step in each bunch had a wider terrace behind it. This was a common feature among the four temperature regimes (probably due to step-flow growth during quenching). In regime 3, on average, only one crossing step existed on a terrace region. When a crossing step reached a lower edge of the upper step bunch, a new step was released from the lower step bunch. This did not depend on the terrace width. After a longer annealing, a terrace region 5 μm wide was formed, but there was only one crossing step. On the other hand, plural steps existed in regimes 2 and 4, where step bunching

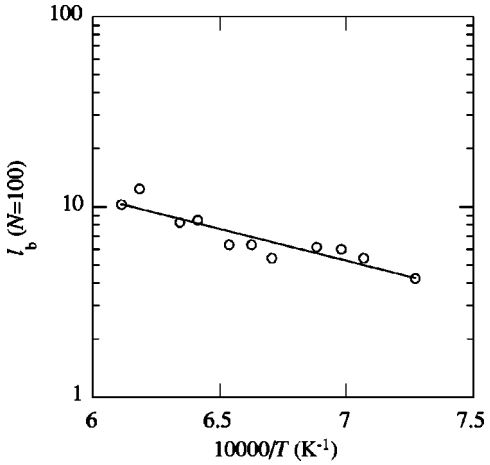

FIG. 5. Temperature variation of the step spacing in a step bunch with 100 steps.

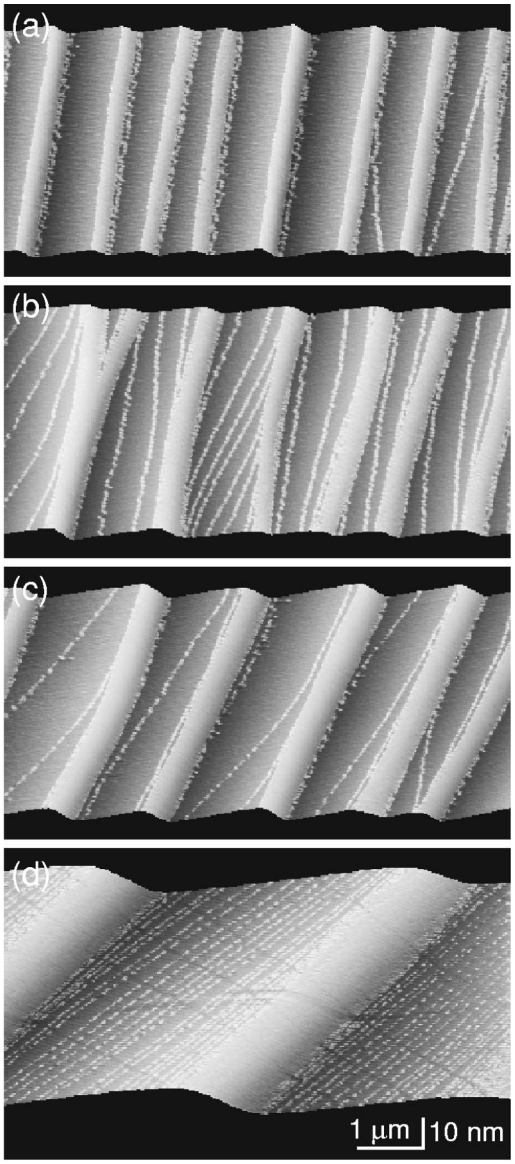

FIG. 6. AFM images of step bunches for the four regimes. (a) Regime 1, created by heating with the step-down current at 910 °C for 4 h. (b) Regime 2, with the step-up current at 1160 °C for 15 min. (c) Regime 3, with the step-down current at 1256 °C for 0.5 min. (d) Regime 4, with the step-up current at 1343 °C for 20 min.

was induced by the step-up current. In regime 2, the step spacing on the terrace region was 30–60 nm, and the number of steps increased with increasing terrace width. In regime 4, though the step-step spacing varied from 10 to 70 nm, the step density was generally much higher than in other regimes.

Sato and Uwaha showed based on their theoretical analysis that the existence of crossing steps is related to the evaporation of adatoms: when evaporation is negligible, no crossing steps exist.[21] Our result in regime 1 corresponds to the negligible evaporation case. However, the difference between regime 3 and regime 2 or 4 implies that evaporation is not the only factor determining the number of crossing steps. There was a distinct difference between the step-down-current case and the step-up-current case. This suggests that the bunching mechanisms are different between these two cases.

IV. DISCUSSION

It is obvious that the scaling exponent changed between two neighboring temperature regimes. In addition, the number of crossing steps on-terrace region changed from one regime to another. Therefore, it is plausible that the bunching mechanism changes when the direction of the bunching-inducing current inverts. In regime 1, bunching is induced by the step-down current. Providing adatoms have a positive effective charge, which is highly realistic, bunching occurs under the step-down force. Thus, this is a typical BCF-type step bunching. Our scaling exponent 0.70 is in good agreement with the theoretical value of $\frac{2}{3}$ derived by Stoyanov and Tonchev for BCF-type bunching with the step-step interaction energy $U=A/l^2$ $(n=2)$.[15] Sato and Uwaha also derived the same exponent for the nonevaporating case.[21] In regime 2, where bunching is induced by the step-up current, the experimental scaling exponent is 0.60. This value is comparable to the theoretical exponent of $\frac{3}{5}$ for transparent steps under the far-from-equilibrium condition, i.e., the adatom concentration n_s in the vicinity of steps is much smaller than the equilibrium concentration n_s^e (here again $U=A/l^2$).[10] Although the transparent-step model did not contradict the experimental results for dc-induced step bunching under the growth condition,[11] the transparency of steps has not been confirmed directly. A difficulty with the transparent-step model is the fact that step-bunching phenomena do not depend on the step orientation. If the transparency is attributed to a small kink density, the kink density should depend on the step orientation. We think that the existence of a wide gap between regimes 1 and 2 is the key to understanding the bunching mechanism. This gap could be a reflection of a gradual change of step properties or adatom transport mechanism. Any model should explain the lack of bunching or very slow bunching in this gap.

In regime 3, step bunching is again induced by the step-down current. The experimental scaling exponent is 0.69. Therefore, this also seems to be BCF-type step bunching. However, the surface in this temperature regime is different from that at lower temperatures. We have shown that the transition between regimes 2 and 3 is accompanied by incomplete surface melting,[22] i.e., disordering of the first monolayer.[23] This is the reason for the abrupt transition from regime 2 to regime 3. However, we do not know the effect of the incompletely melted layer on the step bunching. At least, it is known that atomic steps are preserved underneath the melting layer: step-flow sublimation has been observed even after the transition, and the effective surface diffusion length is about three times larger than that before the transition.[22,24] We assume that the incomplete surface melting is a state with a higher coverage of adatoms. There might be a similar interaction between the adlayer and steps. It is reasonable that steps have a high kink density in such a high-temperature region. Thus, the BCF-type step-bunching model would not contradict the incompletely melted surface.

The step-up current again induces step bunching in regime 4. The scaling exponent is 0.59, which is the same as in regime 2. The transition is rapid: the gap width is less than 30 °C. The transition temperature is the same for both 0.15° and 1° miscut surfaces. This means that the transition does not depend on the step spacing. Misbah, Pierre-Louis, and

Pimpinelli discussed the role of advacancy in step bunching and predicted the reappearance of step bunching when the step spacing is large compared to the adatom diffusion length.[8] Thus, the transition temperature should change for different step spacings in their model. Furthermore, the experimental adatom diffusion length is still as large as 10 μm or more at 1300 °C.[22,24] Therefore, their model cannot be applied without modification. So far, we have not found any structural change at the transition temperature of 1300 °C. It is still possible that advacancies play some role in the transition. Further experimental and theoretical studies are required in order to understand the mechanism of step bunching in this very-high-temperature regime.

The step spacing in a step bunch is a measure of step-step interaction. In the BCF-type model by Stoyanov and Tonchev, the average interstep distance inside the bunch is written as

$$l_b = N^{-2/3}\left(\frac{18aA}{F}\right)^{1/3} B, \tag{1}$$

where a is the distance between atoms along the step edge and B is a constant, which was numerically determined to be 0.63.[15] For regime 2, where step bunching is induced by step-up current, if we adopt the transparent-step model by Stoyanov[10] for far-from-equilibrium evaporation kinetics,

$$l_b = \frac{4}{N^{3/5}}\left(\frac{3}{2\pi^2}\right)^{1/5}\left(\frac{A\lambda_s ab}{F}\right)^{1/5}, \tag{2}$$

where b is the distance between the atoms perpendicular to the step edge and λ_s is the adatom diffusion length. Thus, the relationship between l_b and F/A is highly model dependent. In addition, a model valid in regime 4 has not been established. Hence, we technically calculated F/A using Eq. (1) in regimes 1 and 3 and using Eq. (2) in regimes 2 and 4. The results are summarized in Table I. For Eq. (2), λ_s was set to 10 μm.[22,24] To estimate F values, temperature-dependent A values are necessary. Since experimental A values have been obtained only at around 900 °C, we used the values calculated by Akutsu and Akutsu.[25] They calculated the coefficient of step interaction on the Si(111) ''1×1'' surface for three kinds of short-range order: without short-range order, a $\sqrt{3}\times\sqrt{3}$ short-range order, and a 2×2 short-range order. The degree of temperature dependence changes depending greatly on whether short-range order exists or not. Accordingly, we estimated the degree of temperature variation of A from the result in Fig. 5. If we assume $l_b \sim (A/F)^{1/3}$ like Eq. (1), and the variation of F is small, the slope of the plot in Fig. 5 gives $\frac{1}{3}$ of the ''activation'' energy of A. Then we obtain the ''activation'' energy of $\approx$2 eV (as mentioned in the previous section, this is not an actual energy barrier). In the temperature range from 1160 to 1340 °C, the variation of the values calculated by Akutsu and Akutsu corresponds to an ''activation'' energy of 1.3 eV for the case without short-range order, and 0.3 eV for the $\sqrt{3}\times\sqrt{3}$ or 2×2 short-range order cases. Thus, we adopted the greater-temperature-dependence case, i.e., the case without short-range order, and show the A values in Table I.

For regions 1 and 3, the experimentally determined F/A value is $\approx 1\times10^{-7}\,\mathrm{nm}^{-2}$. Since the electric field was 7 V per 1.7×10^{-2} m, $\approx 4\times10^{2}\,\mathrm{V\,m}^{-1}$, the effective adatom charge was $z_{\mathrm{eff}}\approx 0.1|e|$, where e is the charge of an electron. There was no significant difference in z_{eff} between regimes 1 and 3. The present value is in reasonable agreement with the adatom charge obtained by first-principles calculation (without the wind force), $0.05|e|$.[9] If we use an experimental A value of 0.01–0.04 eV nm at 900 °C,[26] $z_{\mathrm{eff}} \approx 0.02|e| - 0.06|e|$. These values may be slightly larger than the charge estimated from the decay of step bunches by Fu *et al.* ($\leqslant 0.01|e|$).[27] However, considering that their estimation depended on the ratio of adatom diffusion and the attachment/detachment rates to steps, the discrepancy is not significant at all. In regime 2, the transparent-step model gave a large F/A value, $\approx 2\times10^{-6}\,\mathrm{nm}^{-2}$, and a large z_{eff}, $7|e| - 9|e|$. In regime 4, the same model gave smaller values, $F/A \approx 2\times10^{-7}\,\mathrm{nm}^{-2}$, and $z_{\mathrm{eff}} \approx 0.3|e| - 0.6|e|$. Although these values depend on the estimated value of A, the transparent-step model always gave a one order of magnitude larger z_{eff} in regime 2. These values seem unrealistic. So the perfect transparency of steps is not relevant, even though the experimental scaling exponent agrees with the transparent-step model. Fujita, Ichikawa, and Stoyanov also pointed out the same problem.[16]

V. CONCLUSION

We have investigated direct-current-heating-induced step bunches in four temperature regimes above the 7×7-''1×1'' transition temperature. There were distinct differences between the step-down-current-induced bunching (regimes 1 and 3) and the step-up-current-induced bunching (regimes 2 and 4). The scaling exponents of the bunch size were 0.7 for the step-down-current-induced bunching and 0.6 for the step-up-current-induced bunching. The numbers of crossing steps on the terrace region between bunches were zero in regime 1 and 1 in regime 3, while the number increased with increasing terrace width in regimes 2 and 4. A considerable increase of the step-bunching rate was found around the transition from regime 2 to regime 3, i.e., at around 1200 °C. These results imply that the bunching mechanism changed between step-down-current-induced and step-up-current-induced step bunching. The results in regimes 1 and 3 were consistent with the BCF-type step-bunching model. In regimes 2 and 4, the scaling exponent agreed with the transparent-step model far from equilibrium, but the effective charge of adatoms calculated using the model was unrealistically large.

A key to understanding the bunching mechanism lies in the transitions of the bunching-inducing-current direction. There is a wide gap of about 100 °C between regimes 1 and 2. The transition between regimes 2 and 3 is related to incomplete surface melting. The origin of the transition at 1300 °C between regimes 3 and 4 is still unknown. Theoretical models of step bunching should take the wide gap as well as the transitions into consideration.

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