Experimental quantitative study into the effects of electromigration field moderation on step bunching instability development on Si(111)

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We experimentally studied the effects of a moderated electromigration field on the dynamics of the step bunching process on the Si(111) surface at 1130 °C (regime II) and 1270 °C (regime III). The surfaces with step bunch morphologies were created by annealing vicinal Si(111) at fixed temperatures while the applied electric field E was adjusted for every experiment. Scaling relations, $y_m \sim h^\alpha E^q$, between the slope of a step bunch y_m, step bunch height h, and electromigration field E were experimentally probed. Scaling exponents $\alpha \approx 2/3$ and $q \approx 1/3$ were extracted from the step bunch morphologies created by annealing Si(111) in the regime III (1270 °C), which are in good agreement with the predictions of the generalized BCF theory. Scaling exponents $\alpha \approx 3/5$ and $q \approx 1/3$ were extracted from the morphologies created by annealing in regime II (1130 °C). This result was compared to the scaling relations derived within the frame of the transparent step model, which correctly predicts the formation of the step bunching instability by step-up adatom electromigration. The scaling relation obtained by experiment was found to differ from the model predictions. We measured values of critical electric field (E_{cr}), i.e., minimum electric field required for the step bunching to take place. A relatively weak field of $E > 0.5$ V/cm was found to be sufficient to initiate the step bunching process in regime II. This contrasts with regime III, where $E_{\mathrm{cr}} = 1.0$ and 2.0 V/cm were measured for Si miscut from the (111) plane by 1.1° and 2.5°, respectively. The increased values of E_{cr} were attributed to the enhanced step-step repulsion in regime III. The theoretically predicted formation of compressed step density waves was observed upon annealing in both regimes with $E < E_{\mathrm{cr}}$.

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I. INTRODUCTION

The evolution of crystalline vicinal surfaces and the dynamics of atomic steps have long been a topic of great scientific interest.[1] The unique step bunching on the Si(111) surface, has, in particular, been a subject of intense theoretical and experimental studies. Furthermore, the arrays of flat Si(111) terraces separated by closely bunched straight steps can be used as a template for highly ordered nanoscale structures and devices.[2,3]

The step bunching on Si(111) is induced by means of an electric heating current passed through the sample and is driven by the surface electromigration of Si adatoms in the direction of the current flow.[4] This was first reported by Latyshev *et al.* who also found that the final state of a bunched surface depends on the current direction.[5] Currently there are four recognized temperature regimes where step bunching of the Si(111) surface occurs. In the temperature regimes I (∼850–950 °C) and III (∼1200–1300 °C), bunching takes place only if the heating current flows in the step-down direction. A reversal of the current direction is necessary for regimes II (∼1040–1190 °C) and IV (>1300 °C) such that bunching takes place only if the current flows in the step-up direction.[5,6] The limits of the temperature intervals for each regime vary at most by 50 °C in literature.[7]

The reversals of the current direction required to induce step bunching between different temperature regimes are believed to originate from temperature-dependent changes in the "transparency" (permeability) of atomic steps to the flow of Si adatoms, which is determined by the kink density within the steps.[8] The steps are said to be nontransparent when the kink density is high and adatoms easily migrate along the step edges and attach to the kink positions. The steps are assumed to be nontransparent in the generalized Burton-Cabrera-Frank (BCF) theory,[9,10] which predicts that step bunching takes place for the step-down adatom electromigration (regime III).[11,12] Contrary to this, the steps are described as transparent when the density of kinks is low and most adatoms cross the steps without taking part in the exchange between the crystal phase and a surface adlayer.[13] The step bunching in the transparent steps model takes place for the step-up adatom electromigration (regime II).[14,15] This model also predicts that in the presence of net deposition, a reversal of current direction from step up to the step down is required in order to induce a step bunching instability.[16] This was in agreement with earlier experimental studies,[16] but was not observed in subsequent experiments.[17]

Other theories cannot be entirely excluded. For example, it has been shown that transparent steps and steps with fast attachment kinetics cannot be distinguished from each other and both exhibit a stability inversion in the sublimation regime.[18] Another model assumes that different diffusion rates exist in the terrace and step regions, due to local differences in surface reconstruction and bonding. Adatom diffusion is enhanced in the step region and the surface stability reversal is described via negative step kinetic coefficients.[19]

In this paper we concentrate on step bunching as described by transparent[15] and nontransparent step models.[11,12,20] A scaling relation

$$l_{\min} \sim N^{-\alpha}(A/F)^q \quad (1)$$

was derived within the framework of these models, where $l_{\min}$ is the minimum terrace width in the bunch, N is the number

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of steps in a bunch, α and q are positive scaling exponents, $F \equiv q_{\rm eff} E$ is the electromigration force applied to the adatoms, $q_{\rm eff}$ is the Si adatom effective charge, and E is the applied electric field. Constant A in relation (1) is the strength of the entropic and stress mediated repulsion between atomic steps in the equation for the interstep repulsion energy $U = A/l^n$, where l is the interstep distance. The scaling exponents α and q depend on the exponent n and have different values for transparent and nontransparent steps. They can be determined experimentally by measuring the $l_{\rm min}(N)$ and $l_{\rm min}(F)$ dependences and fitting them to a power law. This makes electromigration-induced step bunching a valuable tool for studying the fundamental mechanisms of adatom diffusion and the distance dependence of the repulsive interaction between atomic steps.

The theoretical size scaling relation $l_{\rm min} \sim N^{-\alpha}$ has been tested with experimental results[21,22] and $\alpha = 0.60 \pm 0.04$ and $\alpha = 0.68 \pm 0.03$ were reported[21] for the temperature regimes II (1145 °C) and III (1250 °C), respectively. These values were in excellent agreement with $\alpha = 3/5$ as calculated for bunches of transparent steps under far-from-equilibrium sublimation conditions[15] and $\alpha = 2/3$ as calculated for bunches of nontransparent steps.[11,12] The values of α were, in both cases, calculated for $n = 2$,[23] as is generally accepted, in the expression for the step-step repulsion energy, i.e., $U = A/l^2$. Other experimental studies used the scaling relationships for $l_{\rm min}$ to investigate the temperature dependence of the step interaction coefficient[24] or to estimate the Si adatom effective charge[21,22] and the kinetic length.[25]

Although these models have been widely used in the analysis of step bunching experiments, the scaling relation $l_{\rm min} \sim (1/F)^q$ derived from these models remains untested, although a qualitative study of the influence of a moderated F on $l_{\rm min}$ was recently reported.[26] The critical values of electromigration field ($E_{\rm cr}$), i.e., the minimum electric field required to initiate the step bunching process, also remain unknown. Determining $E_{\rm cr}$ is essential, because it is dependent on A in Eq. (1), which is related to the fundamental thermodynamic quantity $g(T)$, which is in turn associated with the contribution of step-step repulsion to the surface free energy of vicinal crystal surfaces.[27,28] Nevertheless, $E_{\rm cr}$ has not been measured nor has its dependence on temperature and interstep distance on the surface been studied.

In this study we investigate the effect of the electromigration force F on the step bunching process in the temperature regimes II (1130 °C) and III (1270 °C). The design of the annealing setup provided independent control of the radiative and direct current heating.[26] This allowed us to study the step bunching process in a manner that could not be probed in conventional experiments, specifically changing the electric field, while keeping the sample temperature constant. We present the step bunch morphologies obtained on Si(111) at fixed temperatures but with different applied electric fields E. We report the $l_{\rm min}(E)$ and $l_{\rm min}(N)$ dependences obtained from the maximum slope of the step bunches, extract the force and size scaling exponents q and α, and compare them to the predictions of theoretical models. Finally, we report the values of critical field $E_{\rm cr}$ in the annealing regimes II and III for different values of the initial interstep distance determined by the surface miscut angle.

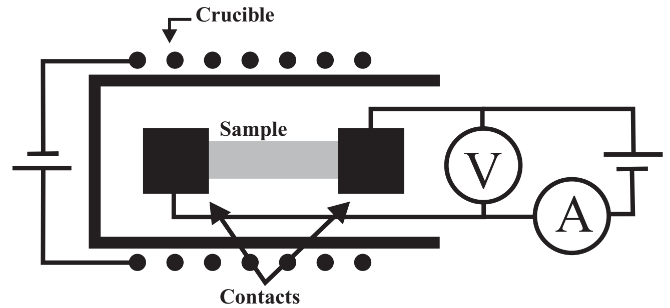

FIG. 1. Schematic of a sample holder inside the crucible. The effects of in-plane applied electric field and sample temperature on step bunching were separated in this way.

II. EXPERIMENTAL PROCEDURE

The experiments were performed at the base pressure of 2×10^{-10} Torr. The step bunch morphology was produced by annealing a series of samples at a fixed temperature, while applying a different voltage to each sample. The maximum applied voltage was attained when the set point temperature was achieved using exclusively dc annealing. Correspondingly, when the entire heating requirement was supplied by the radiative heater, the current driven along the Si(111) and applied voltage were zero.

The $20\times1.5\times0.525$ mm^3 rectangular strips were cut from vicinal Si(111) n-type doped wafers (resistivity ∼1 Ω cm) with a misorientation angle β of 2.5° or 1.1° towards the [11-2] direction. The miscut direction was always oriented along the strips' long side. The strips were mounted onto a sample holder, between two electrical contacts (Fig. 1), and inserted into the alumina crucible of an effusion cell. The sample temperature was extracted from the sample resistance, using the substrate as a resistance thermometer. The resistance versus temperature dependence was calibrated by heating the sample in the crucible to the desired annealing temperature and measuring the resistance between the contacts by the two-point probe technique. The lead resistance was measured independently at the same temperature and taken into account when calculating the electric field across the sample.

The crucible was gradually heated to 650 °C and outgassed for 6 h. Using dc current only, samples were further annealed for 24 h at 450–500 °C and repeatedly flash annealed to 1250 °C for 10 s. The step bunches were formed at 1130 °C by passing a dc current perpendicular to the atomic steps in the step-up direction for 12 h. The current was driven in the step-down direction at 1270 °C. The rate of step bunching at 1270 °C was expected to be nearly two orders of magnitude higher than at 1130 °C, therefore the annealing time was reduced to 6 min.[22] Pressure during the annealing procedure was below 5×10^{-9} Torr. The applied voltage was instantaneously switched off after annealing and the crucible cooled to 650 °C in about 2 min. Such a short thermal annealing did not affect the shape of step bunches.[29] The samples were maintained at 650 °C for 1 h before they were cooled down to room temperature and removed from the UHV for the *ex situ* atomic force microscopy (AFM) characterization.

III. EXPERIMENTAL RESULTS AND DISCUSSION

The step bunching behavior at 1130 °C (temperature regime II) on a Si(111) surface with a misorientation of 2.5° towards the [11-2] direction is summarized in Fig. 2. The figure shows a series of AFM images of step bunch morphologies obtained at different applied electric fields. The surface produced exclusively by the direct current heating ($E = 3.9$ V/cm) is characterized mostly by 3.5–5-μm-wide terraces separated by 1.4–1.9-μm-wide step bunches [Fig. 2(a)]. The step bunches are aligned along the [1-10] direction and cover approximately 25% of surface. As predicted by the scaling relation (1), annealing at a lower applied electric field results in an increased interstep distance and thus the formation of wider step bunches, as shown in Figs. 2(b)–2(e). For example, at $E = 1$ V/cm the width of step bunches is increased to 1.7–2.5 μm while the terrace width is reduced to 2–3.5 μm [Fig. 2(c)]. At $E = 0.9$ V/cm most of the step bunches expand to the size of 3–3.8 μm and account for approximately 70% of the surface area [Fig. 2(d)]. After annealing with $E = 0.6$ V/cm some of the step bunches are no longer separated but spread over the terraces and reach the neighboring bunches [Fig. 2(e)].

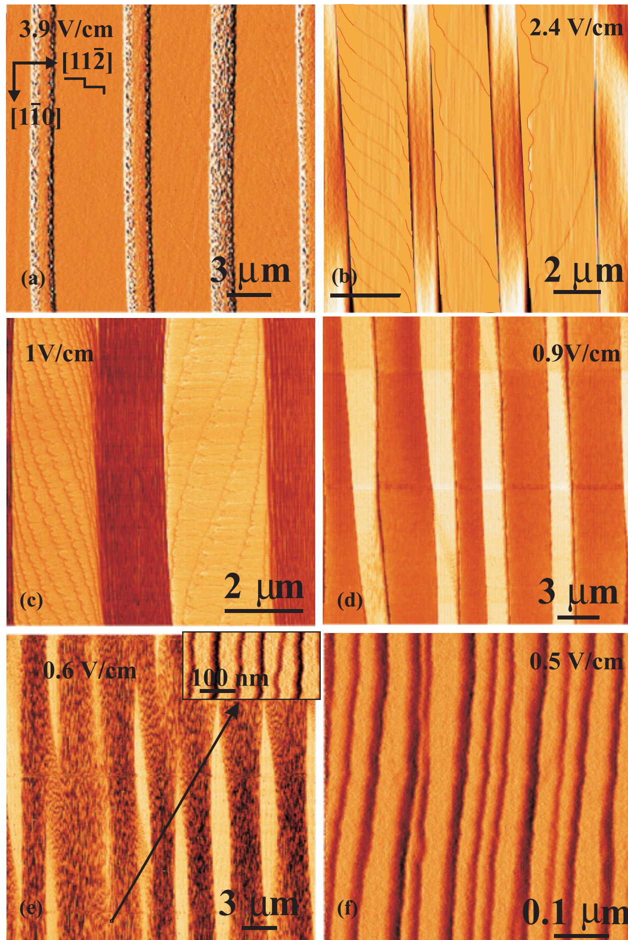

FIG. 2. (Color online) Step bunching morphologies created on Si(111) by annealing at 1130 °C with different applied electric fields. The surface is off cut 2.5° towards the [11-2] direction. The direction of a miscut is from left to right in all images as shown by a stairway sign in Fig. 2(a). Darker areas correspond to step bunches. (a) Differentiated AFM image of a step bunched Si(111) obtained by dc annealing; E= 3.9 V/cm, annealing current I = 2.4 A. (b) Differentiated AFM image of Si(111) after annealing with $E = 2.4$ V/cm, $I = 1.5$ A. (c) Phase AFM image of Si(111) after annealing with $E = 1$ V/cm, $I = 0.6$ A. There is an obvious widening of step bunches as compared to annealing exclusively by dc current. (d) Phase AFM image obtained after annealing with $E = 0.9$ V/cm, $I = 0.55$ A. Most of the step bunches expand to the size of 3–3.8 μm and cover approximately 70% of the surface area. (e) Phase AFM image obtained after annealing with $E = 0.9$ V/cm, $I = 0.4$ A. The step bunches in some areas are still separated by terraces. In other areas they "consume" the terraces and reach the neighboring bunches. (f) Differentiated AFM image of Si(111) after annealing with $E = 0.5$ V/cm, $I = 0.3$ A. The surface appears to be stable against the step bunching when the applied electric field is lower than 0.5 V/cm.

At critical electric field $E_{cr} = 0.5$ V/cm the surface appears to be stable with respect to the step bunching and the formation of a compression step density wave instability is instead observed on the surface [Fig. 2(f)]. A step density wave is generally characterized by a relatively small number of steps in the bunch, which is not affected by the duration of sublimation. At $E = 0.5$ V/cm the electromigration force is no longer sufficient to create coarsening step bunches whose height gradually increases with the sublimation time but the surface is instead characterized by 25–65-nm-wide terraces separated by 1.5–3.5-nm-high step bands (5–12 atomic steps). Annealing with $E = 0.3$ V/cm produced a surface covered by an array of double and triple atomic steps.

The expansion of step bunches with weaker electromigration fields results in a decrease of their slope, so it is convenient to replace the theoretical scaling relation (1) with

$$y_m \sim h^{\alpha} E^{q}, \tag{2}$$

where $y_m = h_0/l_{\min}$ is the maximum slope of a step bunch, $h_0 = 0.314$ nm is a height of a single atomic step, and h is the height of a step bunch given by $h = h_0 N$.[21] Step bunches of different sizes were observed on each sample after annealing and their height (h) was measured with an accuracy of ~1 nm. Mean values of maximum slope y_m were determined for 1 nm intervals of h (similar to the monitoring scheme MS-II in Ref. 30)[30] and $y_m(h)$ was plotted as shown in Fig. 3. The boundaries between step bunches and their adjacent terraces were defined as locations where the bunches' local slope exceeded the surface's global slope, determined by the surface's miscut angle. The $y_m(h)$ data obtained for the same electromigration fields E were fit to a power-law function $y_m = y_0 h^{\alpha}$ and the values of α ranged between 0.57 and 0.59 with a fitting error of ±0.03. This result is in good agreement with $\alpha = 0.6 \pm 0.04$ as was reported in previous experimental studies.[21,22]

The influence of the electromigration force on the slope of step bunches is demonstrated in Fig. 4, which shows cross-sectional profiles along the miscut direction of 208–210-nm-high step bunches produced by annealing with different applied electric fields. From the profiles it is apparent that the slope of step bunches for a given height is gentler for those annealed with weaker electromigration fields, as expected from the scaling relation given by Eq. (2). To attain a quantitative understanding, the maximum slope y_m was plotted against

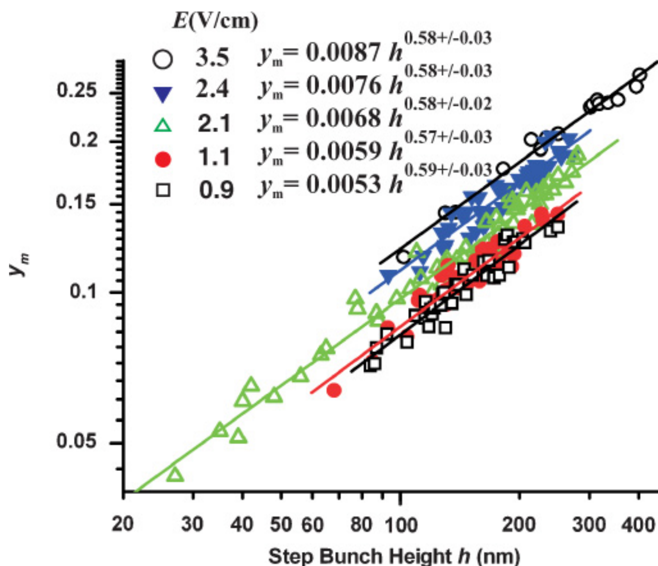

FIG. 3. (Color online) Selected curves of maximum slope y_m versus the step bunch height (h) for vicinal Si(111) annealed at 1130 °C with different electromigration fields E (every fourth experimental point is shown for clarity). The $y_m(h)$ data (E = const) were fit to a power-law function $y_m = y_0 h^{\alpha}$ and values of α ranging between 0.57 and 0.59 were found with a fitting error of ±0.03.

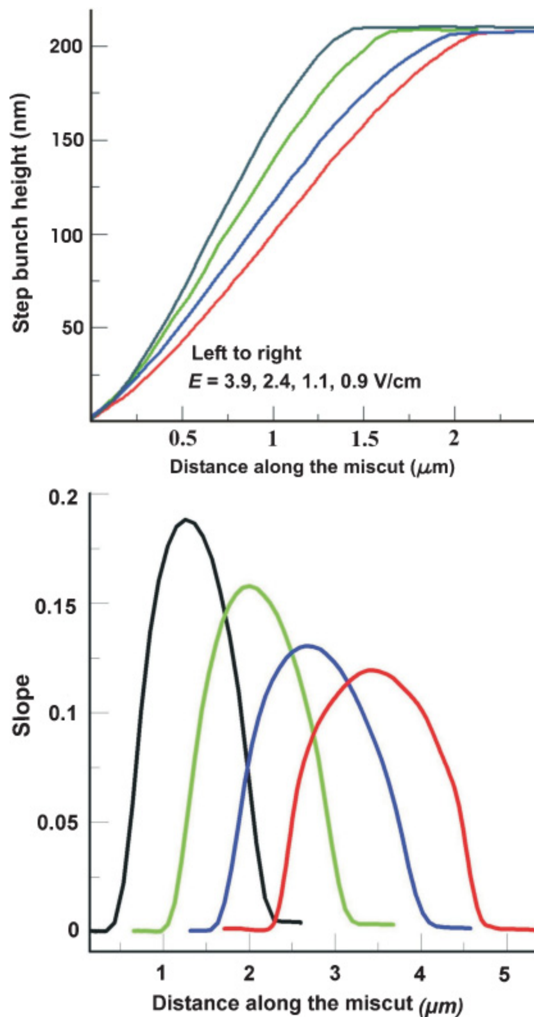

FIG. 4. (Color online) Cross-sectional and slope profiles along the miscut direction of 208–210-nm-high step bunches produced by annealing with different applied electric fields E. The step bunches created by annealing with stronger electromigration fields have steeper slopes.

electromigration field E for different heights of step bunch (Fig. 5). The data were fit to a power-law function $y_m = y_1 E^q$ and the values of q were found to range between 0.32 and 0.35 with an error of ±0.03. The dashed lines in Fig. 5 show the curve fits for data obtained from the calculated scaling equations of y_m as a function of height h (Fig. 3), while the solid lines are the curve fits for data obtained directly from the AFM measurements.

The scaling relationship derived for $U = A/l^2$ ($n = 2$) within the framework of the transparent step model, under far-from- equilibrium evaporation kinetics (i.e., when the adatom concentration in the vicinity of steps is much smaller than the equilibrium concentration), has a form[15]

$$y_m = \frac{1}{4}\left(\frac{2\pi^2 h_0^2 q_{\mathrm{eff}} E}{3A\lambda_s ab}\right)^{1/5} h^{3/5}, \quad (3)$$

where λ_s is the mean diffusion path of adatoms and a and b are the distance between the atoms along and perpendicular to the step edge, respectively. The experimental size scaling exponent $\alpha \approx 0.6$ is confirmed to be in good agreement with the theoretical exponent of $\alpha = 3/5$, however, the experimental value of $q \approx 0.33$ is higher than $q = 1/5$ derived from the model. This value of q, however, is close to $q = 1/3$ as deduced for near-to-equilibrium evaporation conditions using the large h approximation. In this case the scaling relation for y_m is given by equation

$$y_m = \frac{1}{2}\left(\frac{\pi^2 h_0^3 q_{\mathrm{eff}} E D_s n_s^e}{4Ak}\right)^{1/3}, \quad (4)$$

where D_s is the adatom surface diffusion coefficient, k is the step kinetic coefficient, and n_s^e is the equilibrium concentration of adatoms. However, in this situation the model predicts the maximum slope y_m to be independent of the bunch height, which was not the case in our experiment where the $y_m(h)$ dependence followed the $y_m \approx y_0 h^{2/3}$ scaling relation up to the values of $h = 400$ nm, which was the maximum height of step bunches observed on the surface. It is important to point out that Eqs. (3) and (4) were derived by solving a simplified equation for the adatom concentration on a crystal surface. Also, the analytical treatment of the problem is not self-consistent in the sense that the two equations, one describing the bunch shape and the other describing surface diffusion in the bunch region, could not be solved simultaneously, which can be the reason for the observed difference between the experimentally and theoretically obtained scaling relationships.

The step bunching behavior at 1270 °C (regime III) on a Si(111) surface with a misorientation of 1.1° towards the [11-2] direction is summarized in Fig. 6. Similar to temperature regime II, the step bunches widen upon annealing with reduced

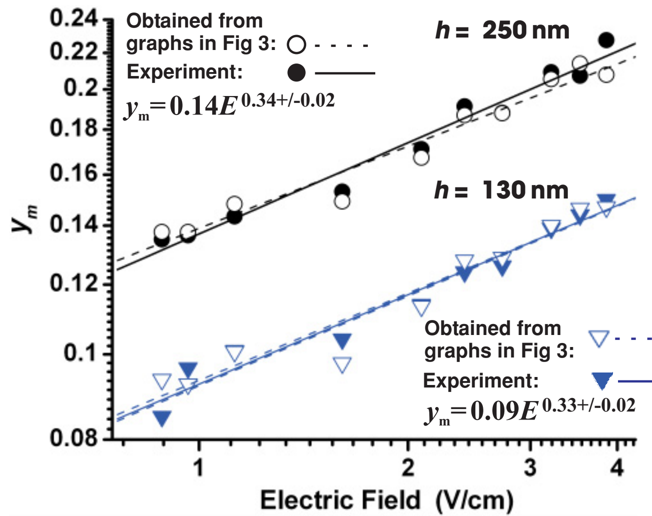

FIG. 5. (Color online) Maximum slope y_m as a function of electromigration field E for 250- and 130-nm-high step bunches. Fitting data to a power-law function $y_m = y_1 E^q$ results in the value of $q \approx 1/3$. Dashed lines show the curve fits for data calculated from the experimentally obtained scaling relations of $y_m = y_0 h^\alpha$ (E = const), while the solid lines are the curve fits for step bunch slopes taken directly from the AFM measurements.

electric fields. Monatomic crossing steps formed on terraces upon annealing at maximum electric field (E =3.6V/cm) are curved in a long-S shape and aligned nearly parallel to the miscut direction. The steady-state S shape of the crossing steps was not achieved due to a relatively short annealing time that was used in the experiment to prevent antiband formation.[31] Weaker electromigration fields create softer gradients of adatom concentration across the terraces[31] and, as a result, the crossing steps gradually elongate in the [1-10] direction and run over a distance of 10 μm or more along the terraces. The relative number of crossing steps and their density are increased with weaker applied fields, which is in agreement with recent theoretical calculations predicting the same result under the weak drift conditions in temperature regimes I and III.[32]

The surface produced by exclusively direct current heating (E = 3.6 V/cm) is characterized mostly by 2.2–3.7-μm-wide terraces separated by 1.0–1.3-μm-wide step bunches [Fig. 6(a)]. In contrast to annealing at 1130 °C, reduction of the electric field resulted not only in the expansion of atomic step bunches and reduction of their slope (Fig. 7) but also in the gradual loss of their straightness [Figs. 6(b)–6(e)]. At E = 1.3 V/cm the width of step bunches increased to 1.2–1.7 μm while the terrace width reduced to 1.5–2.2 μm [Fig. 6(c)]. Figure 6(e) shows a transitional surface morphology observed after annealing with E = 1.1 V/cm, where the step bunching process comes close to cessation. At this field the step bunches expand as far as the neighboring bunches, while flat 0.7–0.8-μm-wide terraces can still be observed in some areas. Annealing with the critical electric field E_{cr} = 1.0 V/cm or weaker created a surface covered by arrays of single, double, and triple steps, as shown in Fig. 6(f). Only single and double steps were observed after annealing with E < 0.8 V/cm.

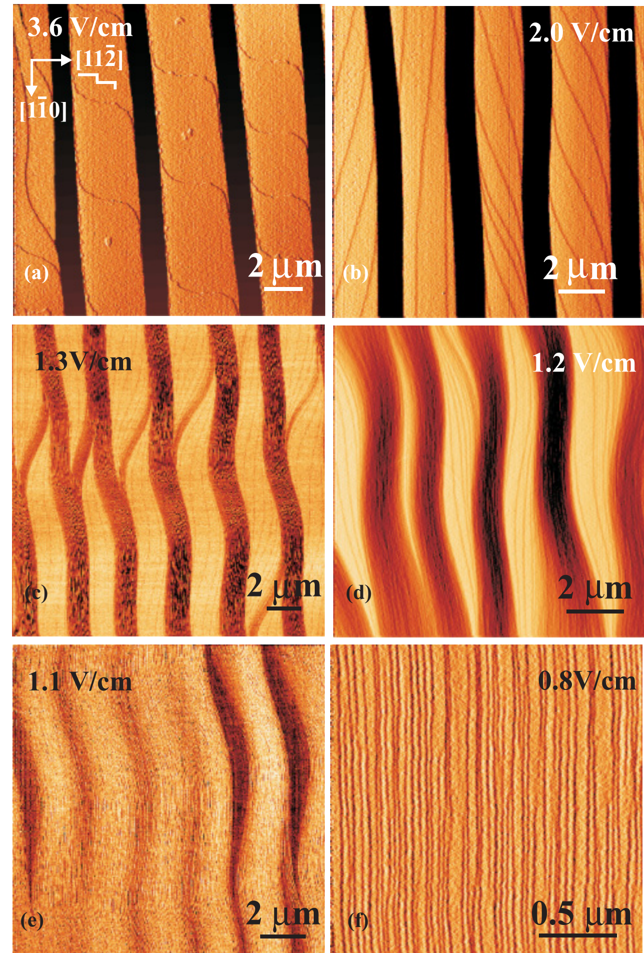

FIG. 6. (Color online) Step bunching morphologies created on Si(111) at 1270 °C by annealing with different electromigration fields. The surface is off cut 1.1° towards the [11-2] direction. The direction of the miscut is from left to right in all images. Darker regions correspond to step bunches. (a) Differentiated AFM image of a step bunched Si(111) surface obtained by dc annealing with E = 3.6 V/cm, annealing current I = 3.8 A. (b) Differentiated AFM image of Si(111) after annealing with E = 2.4 V/cm, I = 2.1 A. (c) Phase AFM image obtained after annealing with E = 1.3 V/cm, I = 1.35 A. (d) Differentiated AFM image obtained after annealing at E = 1.2 V/cm, I = 1.3 A. (e) Phase AFM image obtained after annealing at E = 1.1 V/cm, I = 1.2 A, which shows a transitional surface morphology. Most step bunches expand as far as the neighboring bunches, while flat 0.7–0.8-μm-wide terraces are still present on the surface. (f) Differentiated AFM image obtained after annealing with E = 0.8 V/cm, I = 0.85 A. The surface appears to be stable against the step bunching.

Figure 8 shows the size scaling relation between the maximum slope y_m and the step bunch height h for selected values of applied electric field. The data were fit to a power-law function $y_m = y_0 h^\alpha$ and the size scaling exponents α were found to range between 0.64 and 0.67 with an error of ±0.03, which is in agreement with earlier experimental studies.[21,22] The scaling exponents q ranging between 0.34 and 0.35 with a fitting error of ±0.04 were extracted from the $y_m(E)$ dependence shown in Fig. 9, which was approximated by

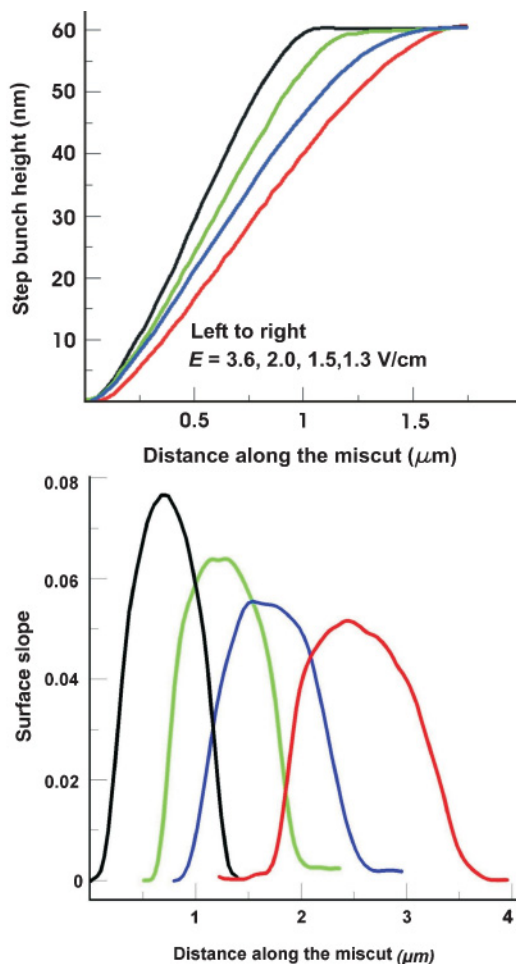

FIG. 7. (Color online) Cross-sectional and slope profiles along the miscut direction of 60-nm-high step bunches produced by annealing at 1270 °C with different applied electric fields E. The step bunches created by annealing with weaker electromigration fields are significantly wider and have gentler slopes.

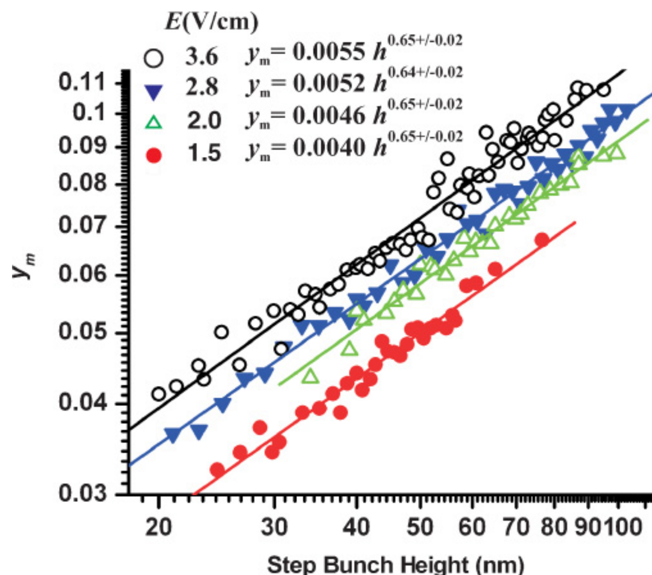

FIG. 8. (Color online) Selected curves of maximum slope y_m versus the step bunch height h for Si(111) surface annealed at 1270 °C with different electromigration fields E. The $y_m(h)$ data were fit to a power-law function $y_m = y_0 h^\alpha$ and values of α ranging between 0.64 and 0.67 with a maximum fitting error ± 0.03 were found (only curves for selected values of E are presented).

relation $y_m = y_1 E^q$. The experimentally determined values of α and q are in a good agreement with $\alpha = 2/3$ and $q = 1/3$ in the scaling relation, obtained within the framework of the generalized BCF theory (nontransparent steps):[11,12]

$$y_m = \frac{1}{B}\left(\frac{h_0 q_{\text{eff}} E}{18aA}\right)^{1/3} h^{2/3}, \tag{5}$$

where B is a constant. The relationship (5) was obtained by solving the continuum model equation for a crystal surface shape with interstep repulsion energy U, given by $U = A/l^2$ $(n = 2)$.[11] The equation was simplified by assuming the absence of adatom desorption and considering the quasiequilibrium shape of a step bunch connecting two infinitely large terraces at different heights. This result is also in agreement with scaling relationships obtained within the framework of the discrete model, which accounts for the adatom desorption.[11] Even with the approximate form of the solution for the crystal shape, the generalized BCF theory well describes the step bunching instability under the influence of electromigration, correctly predicting the shape of step bunches and the scaling relationships between the maximum slope, the electromigration field, and the step bunch height. This is despite an obvious loss of the bunch straightness observed in our experiment for

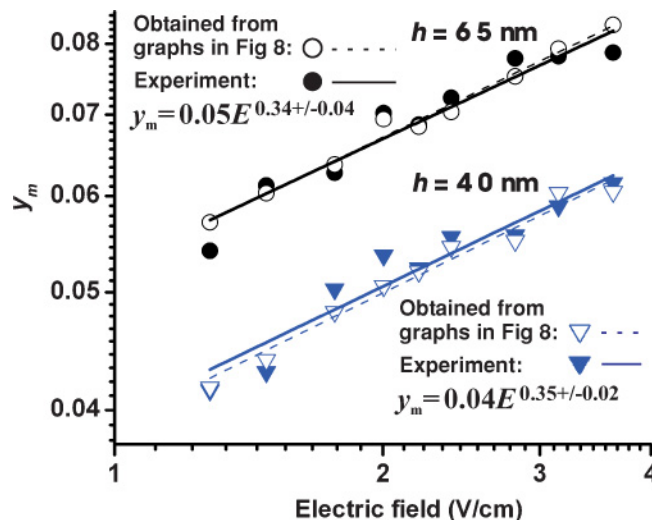

FIG. 9. (Color online) Maximum slope y_m as a function of electromigration field E for 65- and 40-nm-high step bunches. Fitting the data to a power-law function $y_m = y_1 E^q$ results in a value of $q \approx 1/3$. Dashed lines show the curve fits for data calculated from the experimentally obtained scaling equations of $y_m = y_0 h^\alpha$ $(E = \text{const})$; solid lines are the curve fits for step bunch slopes taken directly from the AFM measurements.

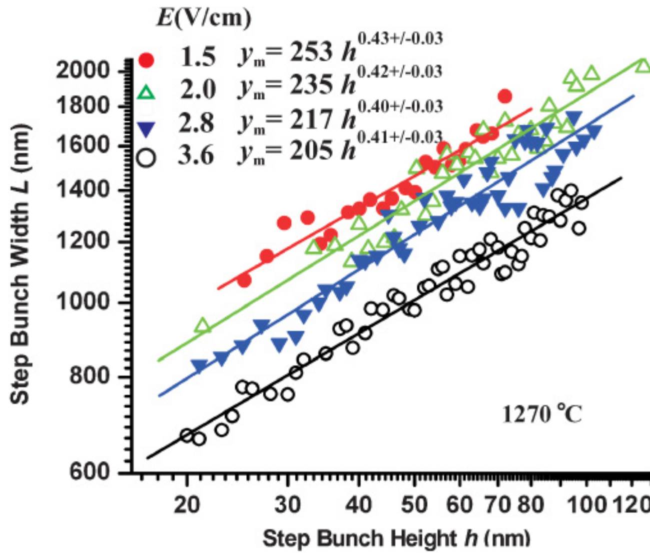

FIG. 10. (Color online) Selected curves of step bunch width L versus the step bunch height h for Si(111) surface annealed at 1270 °C with different electromigration fields E. A power-law fit to the data yields $L \sim h^{0.42\pm0.03}$.

the lower values of E, while the one-dimensional straight step model is employed in the theory.

Numerical integration of step motion equations for the BCF-type step bunching is more reliable and gives similar scaling relations. At the same time, it predicts that the $y_m(E)$ dependence follows the $y_m \sim E^{0.31}$ relation only above the electromigration field defined as $(q_{\rm eff}El/k_BT) = 10^{-5}$, where T is an absolute temperature, k_B is the Boltzmann constant, and l is the initial interstep distance on the crystal surface. For $10^{-6} < (q_{\rm eff}El/k_BT) < 10^{-5}$ the $y_m(E)$ dependence is given by the relation $y_m \sim E^{0.05}$. For the critical electromigration field $E_{\rm cr} = 1.0$ V/cm, $l = 16$ nm and $q_{\rm eff} = (0.05 - 0.35)|e|$,[21,22,33] the parameter $(q_{\rm eff}El/k_BT)$ equals $(0.3 \div 1.8) \times 10^{-6}$ (however, the predicted weakening in the $y_m(E)$ dependence was not observed), and the $y_m \sim E^{1/3}$ relationship was observed over the whole range of electromigration fields above the critical point.

Additionally, step bunch width (L) was investigated as a function of bunch height (Fig. 10). The power-law fit to the data, of the form $L \sim h^{\alpha 0}$, yielded values of α_0 ranging between 0.40 and 0.43 for the step bunches formed at 1270 °C (fitting error ± 0.03). This is in agreement with the result of $\alpha_0 \approx 0.44$, demonstrating the importance of accounting for the step bunch asymmetry when solving the equation for the step bunch shape.[12] This asymmetry can be clearly noted in the step bunch slope profiles shown in Figs. 4 and 7.

The stronger critical electromigration field ($E_{\rm cr}$) required to initiate the step bunching instability at 1270 °C, could be a result of the enhanced step-step repulsion, arising from changes in the step morphology at higher temperatures. It should also be intuitive that repulsive interstep interaction results in a stronger critical field being required to induce the step bunching process on surfaces with a reduced interstep distance l (surface with a larger miscut angle β). Indeed, the relationship describing $E_{\rm cr}$ derived by the linear stability analysis is given by[27,28,34]

$$E_{\rm cr} = \frac{12abAd_s}{\lambda_s^2 l^3 q_{\rm eff}}, \tag{6}$$

where $d_s = D_s/k$ is a characteristic length. Under crystal-vapor equilibrium $A(T) \sim g(T)$,[12] where $g(T)$ is the step repulsion coefficient in the expression

$$f(\rho) = f(0) + k\rho + g\rho^3 \tag{7}$$

for the surface free energy of a vicinal crystal surface with a density of steps ρ. As a result, the $g(T)$ temperature dependence can be experimentally studied, using the linear relation between $A(T)$ and $E_{\rm cr}$. However, d_s is expected to be different for different temperature regimes and so the values of A can be directly compared only if they are measured in the same temperature regime.

In order to probe the theoretically predicted dependence $E_{\rm cr} \sim l/l^3$ given by Eq. (5), we complemented our results with critical-field measurements for the surface with a misorientation $\beta = 1.1^\circ$ at 1130 °C and a surface with misorientation of $\beta = 2.5^\circ$ at 1270 °C. This also allowed a direct comparison between values of critical field for temperature regimes II and III. For both regimes we observed a notable increase in the critical field required when β was 2.5° as compared to 1.1°. When the temperature was changed from 1130 °C to 1270 °C at $\beta = 1.1^\circ$, $E_{\rm cr}$ increased from 0.4 to 1.0V/cm and similarly for $\beta = 2.5^\circ$, an increase from 0.5 to 2.0 V/cm was observed. The values obtained for $E_{\rm cr}$ show that the theoretically predicted dependence of critical field on the interstep distance [Eq. (6)] is too strong to account for the experimental observations on Si(111). Indeed, using the experimental increase of the miscut angle from 1.1° ($l = 15.6$ nm) to 2.5° ($l = 6.9$ nm), the predicted $E_{\rm cr}$ should increase by nearly a factor of 12. Instead, the observed values of $E_{\rm cr}$ increased by approximately a factor of 2 at 1270 °C and only a factor of 1.25 at 1130 °C suggesting a $1/l$ or weaker dependence for $E_{\rm cr}$ depending on the annealing temperature regime.

Morphologies created on surfaces with $\beta = 2.5^\circ$ upon annealing with $E < E_{\rm cr}$ demonstrate that the electromigration field has an effect on the step dynamics even when its strength is below the critical strength for both step-up and step-down adatom diffusion. Annealing at E close to $E_{\rm cr}$ created step density waves composed of 5–12 atomic steps but this number was reduced in weaker electromigration fields. Similar behavior was obtained by numerical integration of the step dynamics equations taking into account a delay in establishing the steady-state concentration of adatoms on atomic terraces ("kinetic memory effect").[27,28] This numerical analysis predicted the formation of step density waves containing 2–3 atomic steps at weak or zero electromigration with the number of steps in the wave increasing for $0 < E < E_{\rm cr}$. This prediction is qualitatively correct, however, we found that only monatomic steps formed on the surface after annealing at zero applied field. In addition, only double and triple steps were created at $E_{\rm cr}$ and below it on the surfaces with misorientation of 1.1°, suggesting that the initial interstep distance should be

taken into account when modeling surface instability below critical field.

IV. CONCLUSIONS

We investigated the effect on the step bunching instability on Si(111) when annealing with the moderated electromigration field. Experimentally observed step bunch morphologies were compared to the predictions of theoretical models. The surface topography in these models is determined by the direction of the adatom electromigration relative to the atomic steps (step up versus step down), strength of the applied electric field E, atomic step "transparency" to the drifting Si adatoms, sublimation conditions, and the form of the relationship between the interstep repulsion energy U and the interstep distance l. The difference in the end state of the step bunched morphologies is expressed in terms of the scaling relation $y_m \sim h^\alpha E^q$ between the slope of a step bunch y_m, step bunch height h, and electromigration field E. We experimentally probed this scaling relation by annealing vicinal Si(111) (miscut towards the [11-2] direction) at fixed temperatures while adjusting the electric field applied along the miscut direction. Temperature regimes II (1130 °C) and III (1270 °C) were investigated, where the step bunching takes place under the influence of step-up and step-down electromigration, respectively. Scaling exponents $\alpha \approx 2/3$ and $q \approx 1/3$ were extracted from the step bunch morphologies created upon annealing Si(111) in regime III (1270 °C). This closely matches morphology predicted by the generalized BCF theory, where atomic steps are assumed to be nontransparent to the migrating Si adatoms and the interstep repulsion energy is inversely proportional to the square of the interstep distance ($U = A/l^2$).

Scaling exponents $\alpha \approx 3/5$ and $q \approx 1/3$ were extracted from the step bunch morphologies created by annealing in regime II (1130 °C). This result was compared to the morphology attained within the frame of the transparent step model, which correctly predicts formation of the step bunching instability by the step-up adatom electromigration. However, the theoretically and experimentally obtained scaling exponents were found to be different. Further theoretical studies are needed in order to explain the mechanism of step bunching instability induced by the step-up electromigration.

We probed the behavior of critical electric field E_{cr}, i.e., the minimum electric field required to initiate the step bunching process. It was found that in regime II the step bunching takes place at a relatively low applied electric field and values of $E_{cr} = 0.4 - 0.5$ V/m were measured. A 2.5–4-fold increase in E_{cr} was recorded, with the switch to regime III (when temperature was changed from 1130 °C to 1270 °C). Such a dramatic increase in E_{cr} was attributed to the enhanced step-step repulsive interaction arising from the changes in the step morphology at higher temperatures. Also a strong dependence of E_{cr} on an average initial interstep distance (l) was recorded in regime III when $E_{cr} = 1.0$ and 2.0 V/m was measured on Si(111) with $l = 15.6$ and 6.9 nm, respectively. This contrasts with regime II where only a very weak dependence of E_{cr} on l was detected. This is an interesting experimental result indicating that different mechanisms are responsible for the step bunching in the case of step-up (regime II) and step-down (regime III) electromigration.

The surface morphology created by annealing with an electric field weaker than E_{cr} was qualitatively investigated. Annealing Si(111) with a misorientation of 2.5° resulted in a formation of compressed step density waves composed of 5-12 atomic steps. This number reduced to 2–3 atomic steps for weaker electromigration fields. Only double and triple steps formed at $E < E_{cr}$ on surfaces with a lower miscut angle of 1.1°.

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