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Properties and dynamic interaction of step density waves at a crystal surface during electromigration affected sublimation

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Electromigration affected sublimation is a complicated phenomenon, involving surface transport coupled to a process of atom exchange between the two-dimensional gas of adatoms and the crystal phase. The case of intensive exchange is theoretically treated and equations of step motion are derived for the case of ''nontransparent'' steps (kinetics with local conservation of adatoms). The numerical integration of these equations manifests step bunching (a formation of step density waves) at step-down direction of the electromigration of adatoms. We studied some properties of the step density waves: the amplitude (the maximum slope of the bunch) and its dependence on the number of steps in the bunch, the kinematic wave velocity and the dynamic interaction of waves of different amplitudes. The central result of this work is the dependence of the minimum interstep distance (in the steady state shape of the bunch) on the model parameters. This dependence, extracted from numerical study, is presented in terms of scaling laws $l_{\mathrm{min}} \sim N^{-r}(A/F)^q$, where N is the number of steps in the bunch, A is the magnitude of step-step repulsion, and F is the force, inducing electromigration of the adatoms. Both scaling exponents r and q depend on the power n in the step-step repulsion dependence on the interstep distance ($U=A/l^n$) and, therefore, they are a key to the problem of experimental evaluation of n. A striking result of this model is the constant value of l_{min} in a wide range of values of the average diffusion distance λ_s . Thus one cannot relate the temperature dependence of l_{min} to the temperature dependence of λ_s . Numerical analysis of the dynamics of steps at a crystal surface of small misorientation angle reveals two types of dynamic interaction of bunches of steps: ''bunch size exchange'' and ''effective coalescence.'' The former type of interaction is rather interesting — a smaller (and faster) bunch approaches a larger one and they travel together until the initially larger bunch achieves (by losing steps) a size, smaller than the size of its partner, and runs away of it. [S0163-1829(98)03227-5]

I. INTRODUCTION

The discovery of the direct current heating effect on the surface morphology of Si wafers revealed a new pathway to study the properties of crystal surfaces. Contrary to the classical studies of surface shape evolution, driven by the reduction of the surface free energy, here we deal with a shape evolution governed by an external driving force—the easy to measure and control electric current flowing through the wafer. In 1989 Latyshev and co-workers[1] reported an interesting effect—the step configuration at a vicinal surface of Si crystal depends on the direction of the heating current, flowing through the crystal. At the step-up direction of the heating current step bunching occurs in the temperature intervals 1050°−1250° and 1350°−1400 °C, whereas at step-down direction of the current bunching occurs in the interval 1250°−1350 °C. Rearrangement of the regular steps into step bands is a reversible process, i.e., changing the specimen temperature beyond the step bunching temperature range or reversing the heating current direction one can transform the developed step bands into a regular system of steps. Later, the effect of direct current heating on the Si(111) surface structure was observed in many experiments.[2–6] Williams *et al.*[4,5] reported step bunching at step-down direction of the current for the temperatures 945 °C and 1245 °C, whereas a formation of step bunches at step-up current takes place at 1190 °C. The STM studies of the dc (direct current) induced bunching of steps produced quantitative data for the time evolution of the wide terraces, separating the bunches, as well as for the interstep distance in the bunch (this distance depends on the number of steps in the bunch). The rate of thermal decay of step bunched structures has been measured in both experiments using an indirect heating source and experiments using direct current in the ''uphill'' direction (the latter stabilizes the equidistant step distribution at a temperature of 930 °C, used in these experiments).[7,8] Interesting experiments on step bunching, induced by alternating heating current of very low frequency have been reported by Metois and Audiffren.[9]

An attempt to describe the effect of the direct current heating on the morphological stability of vicinal surfaces during sublimation was based on a modification[10–13] of the standard Burton-Cabrera-Frank (BCF) diffusion equation

$$D_s \frac{d^2 n_s}{dx^2} - \frac{D_s F}{kT}\frac{dn_s}{dx} - \frac{n_s}{\tau_s} = 0. \qquad (1)$$

This equation describes the diffusion, electromigration, and desorption of the adatoms, adsorbed on the crystal surface [$n_s(x)$ is the concentration of adatoms and τ_s is the average lifetime of an atom in the state of mobile adsorption before leaving the crystal surface] and assumes the hypothesis that a constant electric force F acts on adatoms and induces an average velocity $v = D_s F/kT$, where D_s is the surface diffusion coefficient, k is the Boltzmann constant and T is the

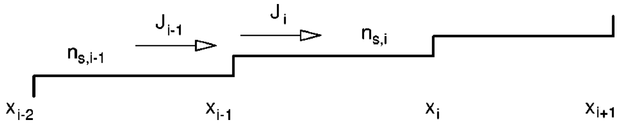

FIG. 1. A vicinal surface with a positive slope. The coordinate of the ith step is denoted by x_i, whereas $n_{s,i}(x)$ and $J_i(x)$ are the adatom concentration field and the adatom flux on the ith terrace [the terrace between the $(i-1)$st and the ith step].

temperature. The surface flux and the adatom concentration in the vicinity of the steps are related by the equations[13]

$$D_s\left(-\frac{dn_{si}}{dx}+\frac{Fn_{si}}{kT}\right)=\begin{cases}-\dfrac{\beta_u}{ab}\,\dfrac{n_{si}-n_s^e(x_{i-1})}{n_s^e(x_{i-1})}, & x=x_{i-1} \quad (2)\\[2ex] \dfrac{\beta_d}{ab}\,\dfrac{n_{si}-n_s^e(x_i)}{n_s^e(x_i)}, & x=x_i, \quad (3)\end{cases}$$

where x_i is the position of the ith step (see Fig. 1), β_u and β_d are the step kinetics coefficients, describing the atom exchange (taking place at each step) between the crystal phase and the two-dimensional gas of adatoms on the higher and lower terrace, respectively, the product ab is the area of one atomic site, $n_{si}(x)$ denotes the concentration of adatoms on the terrace between the $(i-1)$th and the ith step (i.e., on the terrace between x_{i-1} and x_i). Because of the step-step repulsion, the equilibrium concentration $n_s^e(x_i)$ depends upon the distances to the neighboring steps (the calculations are restricted to the interaction between nearest-neighbor steps) , according to the expression[13]

$$n_s^e(x_i)=n_s^e\ \exp\left[-\left(\frac{l_0}{x_{i+1}-x_i}\right)^{n+1}+\left(\frac{l_0}{x_i-x_{i-1}}\right)^{n+1}\right], \tag{4}$$

where

$$l_0=\left(\frac{nabA}{kT}\right)^{1/(n+1)} \tag{5}$$

is a characteristic length, related to the step-step repulsion and n_s^e is the concentration of atoms, adsorbed on a vicinal face of constant interstep distance $(x_{i+1}-x_i=x_i-x_{i-1})$, during crystal-vapor equilibrium. The calculations of the entropic and stress-mediated repulsion between the steps are summarized in Ref. 14 and the resulting interaction energy per unit length of the step is described by

$$U=A/l^n, \tag{6}$$

where l is the interstep distance, the value $n=2$ is shown to be relevant for both entropic and stress mediated repulsion, and A is estimated to be around 0.2 eV Å. The right hand side of the boundary conditions slightly differs from the previous treatment[28]—we take the relative undersaturation at the particular step, so that the denominator is a function of the widths of the two neighboring terraces [see Eq. (4)]. We do not expect this feature of the model to have any significant effect on the step dynamics.

Equations (2) and (3) reflect the silent assumption for an absence of any correlation between the adatom concentrations on neighboring terraces. As seen from the Eq. (2) the surface flux at x_{i-1} [on the terrace between the $(i-1)$th and ith step] is related only to the generating power of the $(i-1)$th step. No quantities, characterizing the adatom concentration and surface flux on the neighboring terrace appear in Eq. (2) (in the terminology of Ref. 7 this is ''kinetics with local adatom conservation). In fact, in the limit $F\to 0$ Eqs. (2) and (3) turn into the well-known boundary conditions for the equation, describing the surface diffusion in the BCF model.[15] These boundary conditions were proposed by Chernov[16] to describe the material balance at the step. It is essential to note that the step kinetic coefficient $\beta(\beta_u$ or $\beta_d)$ characterizes the atom exchange between the *crystal* and the adlayer, i.e., all atoms that attach to the step edge and later leave it without joining the crystal in a kink position do not contribute to β. When many atoms behave in this way, the step is ''transparent'' for the migrating adatoms (according to the terminology, proposed in Ref. 7 , this is ''kinetics without local conservation'') and the use of the boundary conditions (2) and (3) is not justified, since the silent assumption for a lack of correlation between the adatom concentration fields on neighboring terraces is violated. In a recent paper[17] the condition for applicability of the boundary conditions (2) and (3) was shown to be

$$(\beta/D_s b n_s^e)=1. \tag{7}$$

To derive this relation one considers the frequency ω_+ of atom attachment (the irreversible detachment of an atom from the crystal during sublimation is not a result of a single act of detachment, but usually it is the final result of many detachments and subsequent attachments of the same atom to the crystal) to a randomly selected atomic site at the step edge. This frequency is equal to $D_s n_s$, which results from the multiplication of the hopping frequency $\nu\ \exp(-E_{sd}/kT)$ and the probability $n_s ab$ to find an adatom at a single jump distance from the selected atomic site at the step edge (n_s here denotes the concentration of adatoms in the step vicinity). It is more complicated, however, to write an expression for the effective frequency of atom attachment to the *crystal*, since this is a result of a sequence of elementary processes (attachment to the step, migration along the step edge, and attachment to a kink). The net number of atoms detached from the crystal during sublimation (per unit length of the step and unit time) as a result of the ''trial and error'' process is given by the right-hand side of Eqs. (2) and (3). To arrive at a dimensionality of frequency one multiplies the right-hand side of the boundary conditions by the length a of an atomic site along the step and gets the net number $(\beta/b)n_s/n_s^e-\beta/b$ of atoms, which an atomic row perpendicular to the step edge loses in unit time (here β is used instead of β_d and β_u since the asymmetry of the step kinetic coefficient is not essential for this consideration; the index i is omitted because of the general validity of the considerations). The net number of atoms, detached per unit time from an atomic row perpendicular to the step can be, formally, at least, considered as a difference between effective frequencies $\omega_{\rm eff}^+$ and $\omega_{\rm eff}^-$ of atom attachment and detachment (one should keep in mind that $\omega_{\rm eff}^+$ and $\omega_{\rm eff}^-$ are not frequencies of real *elementary* processes). Defined in this way, the effective frequencies are given by $\omega_{\rm eff}^+$

$=(\beta/b)n_s/n_s^e$ and $\omega_{\mathrm{eff}}^{-}=\beta/b$. Concerning the physical meaning of the effective frequencies, one can easily see that $\omega_{\mathrm{eff}}^{+}$, for instance, is equal to the number of atoms attached to the crystal (per atomic site and unit time) during the ''trial and error'' process, whose net result is crystal sublimation. Therefore, the equality $\omega_{+}=D_s n_s=\omega_{\mathrm{eff}}^{+}$ means that all atoms attached to the step edge (with a frequency $\omega_{+}=D_s n_s$) migrate along it and attach to a kink position, i.e., the probability for an adatom to cross the step is negligible (the ''transparency'' of the step is zero). This is precisely the condition for applicability of the boundary conditions (2) and (3). Substituting $\omega_{\mathrm{eff}}^{+}$ with $(\beta/b)n_s/n_s^e$ one arrives at Eq. (7). This is a very useful relation, since it provides a ground to decrease the number of the parameters involved in the equations of step motion. Recently, however, Williams pointed out that the basic relation (7) corresponds to the special case where the diffusion constant for binding to the step edge is the same as the diffusion constant for motion between equivalent sites on the terrace (this situation seems close to reality for diffusion on metal surfaces). For semiconductors, however, Williams suggested the reasonable possibility for an additional energy barrier E_{at}, related to the atom attachment to the step edge, i.e., $\omega_{+}=D_s n_s \exp(-E_{\mathrm{at}}/kT)$ and Eq. (7) turns into

$$\frac{\beta}{D_s b n_s^e}=\exp(-E_{\mathrm{at}}/kT). \tag{8}$$

Equations (7) and (8) are not new [Eq. (7) results from Eq. (8) in the limit $E_{\mathrm{at}}=0$], although their derivation from microscopic considerations is original. In their analysis of step motions on high-temperature vicinal surfaces Pimpinelli *et al.*[31] introduced a characteristic length d_s, associated with the attachment kinetics. They derived the temperature dependence of d_s and also explained the physics—instantaneous sticking of adatoms to the step (at kink sites) implies $d_s=a$. Equation (8) in this paper is identical to Eq. (13) in the paper of Pimpinelli *et al.*[31] [the left-hand side of Eq. (8) represents the ratio a/d_s]. Since we are studying the effect of the electromigration on the stability of the crystal surface, the essential property of the steps is their ''nontransparency'' (this term addresses directly the surface transport, induced by electromigration). This property, however, is identical with the ''instantaneous sticking'' discussed in Ref. 31. Let us point out again that the use of a model of BCF class to study the effect of the electromigration is justified in the case of ''nontransparent'' steps (instantaneous sticking of adatoms to the steps). The crystal growth and evaporation kinetics in the case of transparent steps has been addressed by Nozieres[32,33] by advancing a model that does not belong to the BCF class—the rate of motion of a given step does not depend only on the width of the two neighboring terraces, but also on the positions of many other steps (we shall return to the Nozieres model in Sec. IV).

It should be noted that the problem of applicability of the boundary conditions (2) and (3) emerges only in a presence of electromigration. Because of the symmetry of the classical model of Burton, Cabrera, and Frank there is no discontinuity of the adatom concentration and the net flux across the step is zero, irrespective to the intensity of the crystal-adlayer exchange (a discontinuity of the adatom concentration appears, however, in a presence of a Schwoebel effect[18]). The electromigration force breaks the symmetry of the BCF model and reveals new features of the surface transport leading to specific changes of the shape of the crystal surface during sublimation.

The aim of this paper is to study the surface transport in the presence of electromigration of the adatoms and to analyze the resulting changes of the shape of the crystal surface during sublimation. The shape of the step density waves and their dynamic interaction in a regime of morphological instability is studied in detail by numerical integration of the equations of step motion as well as in the framework of the continuum model.

II. EQUATIONS OF STEP MOTION

In this section, the explicit form of the equations for step motion is derived for the regime of electromigration affected sublimation, characterized by strong coupling of the surface transport to the exchange of atoms between the crystal phase and the 2D gas of adatoms on the crystal surface, i.e., when Eq. (7) is satisfied. In this case the diffusion problem on the crystal surface can be reduced to a diffusion problem on a single terrace (since the surface transport is effectively interrupted at each step by the high rate exchange of atoms with the crystal phase). The equations derived below are not valid for the electromigration affected sublimation, characterized by a ''high transparency'' of the elementary steps, i.e., when $(\beta/D_s b n_s^e)\ll 1$.

The equations of step motion in this regime of negligible exchange between the adlayers on neighboring terraces are

$$\frac{dx_i}{dt}=-\beta_u\frac{n_{s,i+1}(x_i)-n_s^e(x_i)}{n_s^e(x_i)}-\beta_d\frac{n_{s,i}(x_i)-n_s^e(x_i)}{n_s^e(x_i)}, \tag{9}$$

where x_i is the position of the ith step, whereas $n_{s,i+1}(x_i)$ and $n_{s,i}(x_i)$ are the actual concentrations of adatoms in the vicinity of the ith step on the higher and the lower terrace (see Fig. 1).

The substitution of the solution of Eq. (1) with boundary conditions (2) and (3) into (9) results in the following equations of the step motion:

$$\begin{aligned}\frac{dx_i}{dt}=\beta_u&\frac{\Psi_{+}(x_{i+1})[1+\gamma_d(x_{i+1})\alpha_{+}]-\Phi_{-}(x_{i+1})2\gamma_d(x_i)\alpha-\Psi_{-}(x_{i+1})[1-\gamma_d(x_{i+1})\alpha_{-}]}{\Psi_{+}(x_{i+1})\varphi_{+}(x_{i+1})-\Psi_{-}(x_{i+1})\varphi_{-}(x_{i+1})}\\&+\beta_d\frac{\Psi_{+}(x_i)[1+\gamma_u(x_{i-1})\alpha_{-}]-\Phi_{+}(x_i)2\gamma_u(x_i)\alpha-\Psi_{-}(x_i)[1-\gamma_u(x_{i-1})\alpha_{+}]}{\Psi_{+}(x_i)\varphi_{+}(x_i)-\Psi_{-}(x_i)\varphi_{-}(x_i)},\end{aligned} \tag{10}$$

where

$$\alpha=\sqrt{1+\left(\frac{F\lambda_s}{2kT}\right)^2},\quad \alpha_+=\alpha+\frac{F\lambda_s}{2kT},\quad \alpha_-=\alpha-\frac{F\lambda_s}{2kT},$$

$$\gamma_u(x_i)=\frac{\beta_u\lambda_s}{D_s abn_s^e(x_i)},\quad \gamma_d(x_i)=\frac{\beta_d\lambda_s}{D_s abn_s^e(x_i)},$$

$$\varphi_+(x_i)=1+\gamma_d(x_i)\alpha_+ +\gamma_u(x_{i-1})\alpha_- +\gamma_u(x_{i-1})\gamma_d(x_i),$$

$$\varphi_-(x_i)=1-\gamma_d(x_i)\alpha_- -\gamma_u(x_{i-1})\alpha_+ +\gamma_u(x_{i-1})\gamma_d(x_i)$$

$$\Psi_+(x_i)=\exp[\alpha(x_i-x_{i-1})/\lambda_s],$$

$$\Psi_-(x_i)=\exp[-\alpha(x_i-x_{i-1})/\lambda_s]$$

$$\Phi_-(x_i)=\exp[-F(x_i-x_{i-1})/2kT],$$

$$\Phi_+(x_i)=\exp[F(x_i-x_{i-1})/2kT].$$

Equations (10) describe the dynamics of steps during sublimation, affected by an electromigration of the adatoms on the crystal surface. These equations provide a ground to study the impact of the Schwoebel effect ($\beta_u\neq\beta_d$), the electromigration of adatoms ($F\neq 0$), and the step-step repulsion ($l_0\neq 0$) on the step distribution at the evaporating surface. Since Eqs. (10) have been derived on the basis of the generalized BCF model [Eq. (1)] and boundary conditions [Eqs. (2) and (3)], their validity is restricted to the region of experimental conditions, where the Eq. (7) is fulfilled (the adatoms on each terrace obey a local conservation condition[7]). The importance of the considerations for the applicability of the generalized BCF model was not realized in the previous papers in the field and the equations of step motion were numerically integrated without taking into account the validity condition (7) (see Refs. 19 and 12). A more complicated model for the step bunching dynamics in the presence of an alternating heating current has been developed by Houchmandzadeh *et al.*,[20] but they also have not realized that the condition of validity of the model implies a relation between the parameters, involved in the equations of step motion [since Eq. (7) should be satisfied].

III. MORPHOLOGICAL INSTABILITY OF VICINAL SURFACE DURING SUBLIMATION

In the numerical integration one handles M equations with the usual periodical condition $x_{M+1}=x_1+Ml$, where l is the average interstep distance, determined by the misorientation angle of the wafer. Neglecting the Schwoebel effect and introducing dimensionless coordinates $\xi_i=x_i/l$ and time $\tau=\beta t/l$, one still has 4 parameters in Eq. (10). Two of them, l/λ_s and $\beta\lambda_s/D_s abn_s^e$, determine the rate of motion of a train of equidistant steps, whereas l_0/l characterizes the step-step repulsion, and $Fl/2kT$ reflects the impact of the electromigration. Now, one can make use of the condition $\beta/D_s bn_s^e=1$ for a validity of the boundary conditions (2) and (3) to reduce the parameter $\beta\lambda_s/D_s abn_s^e$ to λ_s/a. Since a (the interatomic distance) and l are well known parameters in each experiment, selecting values of l/λ_s and $\beta\lambda_s/D_s abn_s^e$ is, in fact, reduced to selecting a value of the mean diffusion distance λ_s .

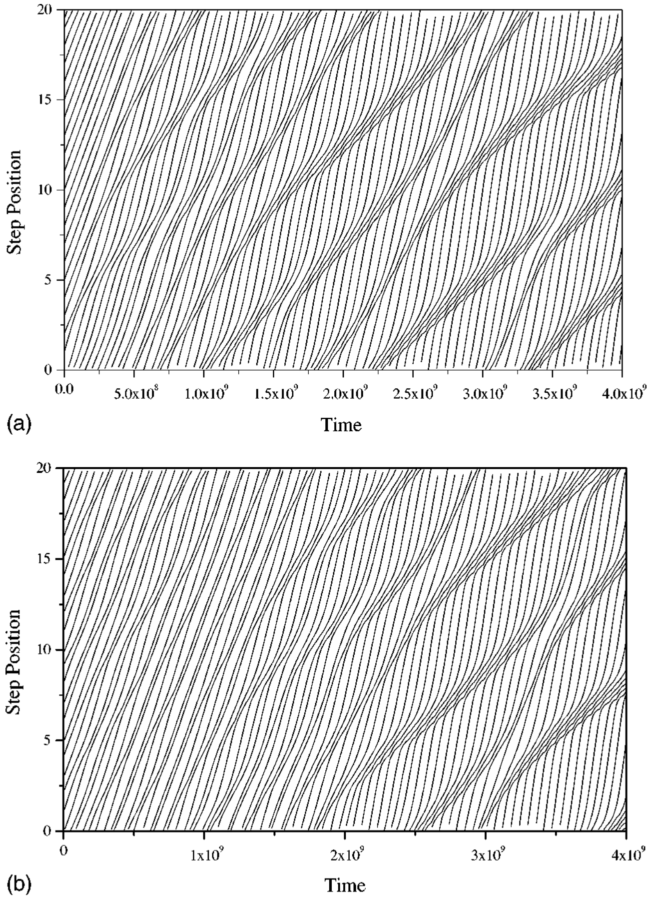

FIG. 2. Trajectories $\xi_i(\tau)$, $i=1,2,\ldots,M$, of the steps during electromigration affected sublimation obtained by numerical integration of the equations of step motion (the values of the dimensionless time τ are not instructive; the physical time corresponds to the evaporation of about 80 ML). The values of the parameters involved in Eq. (10) are $Fl/2kT=-0.000\,06$, $l/\lambda_s=0.0025$, $\beta\lambda_s/D_s abn_s^e=117\,000$, and $l_0/l=0.003$. The initial conditions used to produce (a) are $\xi_i(0)=i,(i=1,2,\ldots,19)$, $\xi_{20}(0)=19.5$, whereas (b) was produced by $\xi_i(0)=i+\Delta\xi_i$ where $\Delta\xi_i$ were produced by random number generator. When the trajectory $\xi_i(\tau)$ exceeds the value $\xi=M$ (the top of the figure) it reappears at $\xi=0$ (the bottom of the figure).

Numerical integration of the equations of step motion [Eqs. (10)] manifests step bunching at the step-down direction of the electromigration of the adatoms, i.e., at $F<0$. The initial stages of step bunching are shown in Fig. 2 for different step configurations at $t=0$. Equidistant step distribution ($\xi_i=i$ at $i=1,2,\ldots,19$) with only one step ($i=20$) deviated from its regular site ($\xi_{20}=19.5$) is used as a starting step configuration in the numerical integration of Eqs. (10), which produces the step trajectories shown in Fig. 2(a). The step trajectories shown in Fig. 2(b) have been obtained when the initial values of ξ_i are $\xi_i=i+\Delta\xi_i$, where the deviations $\Delta\xi_i$ are produced by a random number generator. As seen, a formation of bunches of steps takes place in both cases, as long as the electromigration force F has a step-down direction. When, however, the force F has a step-up direction (i.e., $F>0$) , the numerical integration of the equations of step motion (10) manifests stability of the regular distribution of the steps during sublimation of the vicinal surface.

A. Properties of step density wave

Integrating the equations of step motion one can study the properties of the step density waves at a vicinal surface. The theoretical results could be compared to the experimental observations to get quantitative information about some surface phenomena and some physical quantities, characterizing the steps at the crystal surface. Step bunching, induced by electromigration, is rather promising in this respect, since the interstep distance l_b in the bunch is a result of a sensitive balance between the step-step repulsion and the effect of the force F, inducing electromigration of adatoms. Since l_b is a measurable quantity and, on the other hand, it can be determined by numerical integration of the equations of step motion, it is reasonable to explore this pathway towards extracting values of the magnitude A of the step-step repulsion and the electromigration force F from relevant experiments.

The task of the theoretical treatment is to reveal how l_b depends on the number N_b of the steps in the bunch, on the diffusion distance λ_s, on the magnitude A of the step-step repulsion and the electromigration force F. For this purpose we started the numerical integration of the equations of step motion from an initial surface configuration with only one step density wave [Fig. 3(a)]. After some integration time the step density wave achieved a steady state size (number of steps in the bunch) and shape. Then the minimum interstep distance $l_{\min}$ in the bunch was determined after each integration step and averaged over a considerable period of time [as seen in Fig. 3(b) $l_{\min}$ is an oscillating function of the sublimation time, because of the step detachment from the leading edge of the bunch and step attachment to the bunch tail]. Making use of this procedure we first proved that $l_{\min}$ does not depend on the average interstep distance l (i.e., on the misorientation angle of the wafer). The dependence of $l_{\min}$ on the number N_b of steps in the bunch is shown in Fig. 4 (as seen the numerical results can be approximated by the simple relation $l_{\min}/l \sim N^{-0.68}$). In the numerical integration of Eq. (10) we used the parameter values $Fl/2kT=-0.000\,06$, $l/\lambda_s=0.0025$, $\beta\lambda_s/D_s a b n_s^e=117\,000$, and $l_0/l=0.003$, shown in an earlier paper[17] to reproduce the experimental observations of Williams and co-workers on bunching at 1250 °C. Determining the dependence of $l_{\min}$ on F at a constant N_b is more complicated because the total number M of steps in the system should be appropriately adjusted in each integration run with different value of F, in order to keep the bunch size constant. The results obtained for a bunch consisting of 21 steps are shown in Fig. 5(a). It is of interest to note that the values of the parameter $Fl/2kT$ used in the integration runs, carried out to prepare Fig. 5(a), correspond to values of the effective charge of the adatom ranging from $z_e=0.01$ to $z_e=1.0$ of the elementary electric charge [these estimations refer to a temperature $T=1250$ °C and take into account that the voltage drop across the sample is 5 V/cm, and the average interstep distance is $l=1300$ Å (as in the experiments of Williams[4,5])]. In this way the theoretical data for the dependence of $l_{\min}$ on F covers almost the whole range of values of the effective electric charge of an adatom, reported in various papers (see Refs. 21,22). As seen, the dependence of $l_{\min}/l$ on the electromigration inducing force F clearly shows two branches—for $Fl/2kT>10^{-5}$ the numerical results can be approximated by the relation $l_{\min}/l \sim F^{-0.31}$, whereas in the interval $10^{-6}<Fl/2kT<10^{-5}$ the relation is $l_{\min}/l \sim F^{-0.05}$. Follow-

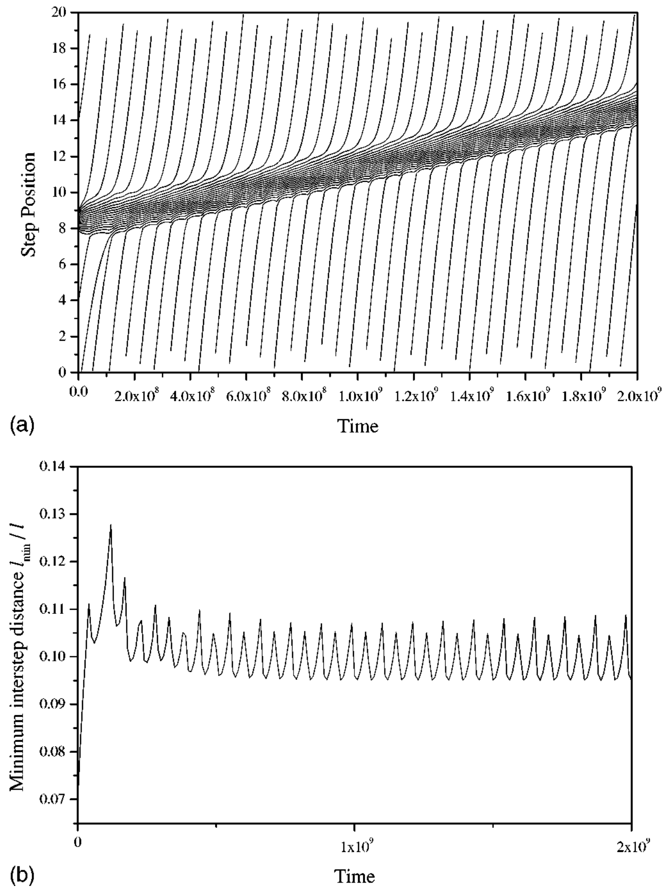

FIG. 3. (a) Trajectories of steps on a crystal surface with a single bunch (a single step density wave). The parameters used in the integration of Eq. (10) have the same values as in Fig. 2. As seen, single steps detach from the front edge of the bunch whereas a process of attachment of fast moving single steps takes place at the opposite edge. (b) The values of the minimum interstep distance $l_{\min}/l$ are plotted against the sublimation time.

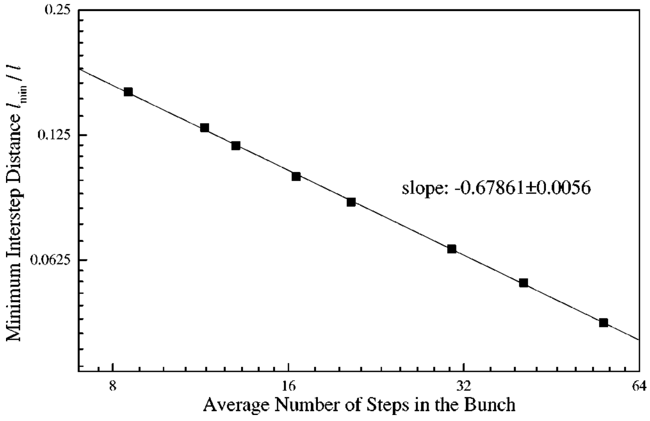

FIG. 4. Minimum interstep distance $l_{\min}/l$ in a steady-state bunch as a function of the number of steps in the bunch. The values of the parameters are the same as in Figs. 2 and 3.

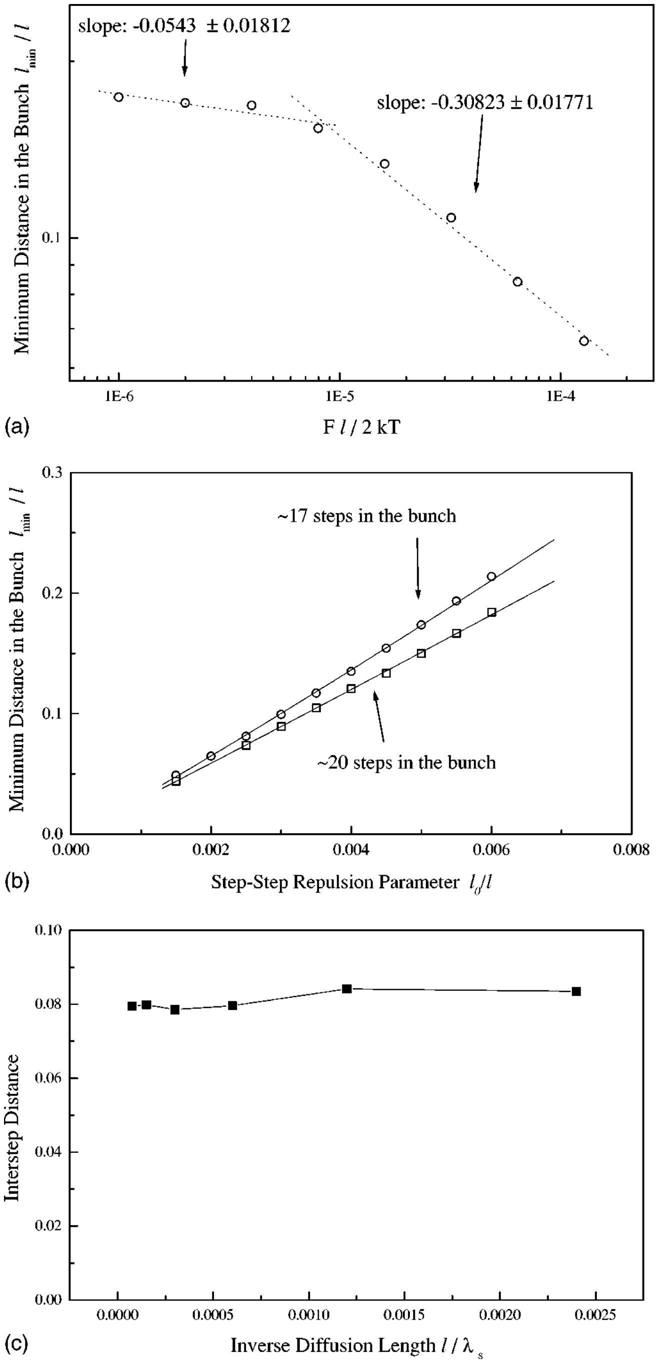

FIG. 5. Dependences of minimum interstep distance in the bunch l_{min}/l on (a) the electromigration force F, (b) the step-step repulsion [the parameter l_0/l is related to the magnitude A of the step-step repulsion by the equation $l_0=(nabA/kT)^{1/(n+1)}$, where $n=2$ is the usual assumption], and (c) the mean diffusion distance λ_s (in the integration runs carried out to obtain the results shown in (c) we used much smaller values of the force $F[Fl/2kT=0.000\,001)]$.

ing the same procedure we determined the dependence of l_{min} on the magnitude of the step-step repulsion, i.e., on the parameter l_0/l. The obtained results, shown in Fig. 5(b), manifest a linear dependence of l_{min} on l_0/l . Having in mind the relations (5) and (6) one can conclude that the dependence of l_{min} on the magnitude A of the step-step repulsion can be described by the expression $l_{\mathrm{min}}{\sim}A^{0.33}$. As seen, the scaling exponent is equal (but having the opposite sign) to that appearing in the scaling relation $l_{\mathrm{min}}(F)$ at $Fl/2kT>10^{-5}$. Here one should note that the values of l_0/l used in the integration of the equations of step motion to produce data for Fig. 5(b) correspond to magnitudes of the step-step repulsion in the range from $A=0.025$ to $A=1.5$ eV Å [see Eq. (6)].

To study the dependence of l_{min} on λ_s we integrated Eqs. (10) using different values of the mean diffusion distance λ_s [in all integration runs we had $Fl/2kT=-0.000\,06$ and $l_0/l=0.003$, whereas in each integration run the parameter l/λ_s was two times larger than in the previous one, and the parameter $\beta\lambda_s/D_s abn_s^e$ was two times smaller in order to satisfy the basic relation (7)]. Thus we obtained an almost constant value $l_{\mathrm{min}}/l=0.12$ in the interval $0.000\,078\leqslant l/\lambda_s\leqslant 0.003$ for a bunch, consisting of 15 steps. The value of l_{min}/l was found to sharply increase with the increase of the parameter l/λ_s when $l/\lambda_s>0.004$. It is essential to note, however, that nucleation of step bunches does not take place at $l/\lambda_s\geqslant 0.005$, i.e., starting the integration of Eqs. (10) from an initial configuration of steps, randomly deviated from their regular positions, we never observed a formation of step density waves.

It is of interest to study the dependence of l_{min} on the mean diffusion distance λ_s in the presence of additional energy barrier for an adatom attachment to a step edge, i.e., when Eq. (8) is satisfied instead of Eq. (7). The activation energy E_{at} for an adatom attachment to a step edge is, in fact, an additional parameter. To get some impression of how the presence of the barrier E_{at} modifies the dependence of l_{min} on λ_s it is convenient to express E_{at} as a fraction of the energy $E_{\mathrm{des}}-E_{\mathrm{sd}}$ (E_{des} is the activation energy for desorption of an adatom from a terrace, and E_{sd} is the activation energy for surface diffusion), which determines the temperature dependence of λ_s ($\lambda_s=a\exp[(E_{\mathrm{des}}-E_{\mathrm{sd}})/2kT]$). Substituting $E_{\mathrm{at}}=\theta(E_{\mathrm{des}}-E_{\mathrm{sd}})/2$ into Eq. (8) one obtains $\beta/D_s bn_s^e=(a/\lambda_s)^{\theta}$ and therefore the parameter $\beta\lambda_s/D_s abn_s^e$ is reduced to $(\lambda_s/a)^{1-\theta}$. Now, for each fixed value of θ, one can calculate the value of the parameter $\beta\lambda_s/D_s abn_s^e=(\lambda_s/a)^{1-\theta}$ provided the value of the parameter l/λ_s is already selected. As an example we assumed $\theta=0.5$ and integrated the equations of step motion for different values of λ_s. The results show the minimum interstep distance l_{min} in the bunch to have again an almost constant value [see Fig. 5(c)] . In these integration runs we used much smaller values of the force F ($Fl/2kT=0.000\,001$) in order to obtain $l_{\mathrm{min}}/l\approx 0.08$ in a bunch of 15 steps, which is close to the experimentally obtained[23] values of the interstep distance in the bunches of this size during sublimation of Si at $T=1250\,^{\circ}\mathrm{C}$. On the basis of the above results we conclude that the model under considerations predicts a constant value of the minimum interstep distance l_{min} in a relatively large range of values of λ_s. The presence of an additional energy barrier E_{at} for adatom attachment to a step edge does not change this conclusion. In the presence of an additional energy barrier, however, much smaller effective electric charge of the adatoms is necessary in order to reproduce the experimentally observed values of l_{min}. Really, the value $Fl/2kT=0.000\,001$ corresponds to an effective charge $z_e=0.004|e|$, whereas $z_e=0.24|e|$ corresponds to the value

$Fl/2kT = -0.000\,06$, used in the integration runs in absence of additional energy barrier for adatom attachment to the step edge (i.e., $E_{\mathrm{at}}=0$).

B. Dynamic interaction of step density waves

To get deeper insight of the surface morphology and the instabilities during electromigration affected sublimation we started the numerical integration of the equations of step motion from an initial surface configuration with two step density waves. The resulting step trajectories, shown in Fig. 6 manifest a solitonlike behavior and two types of dynamic interaction between the step density waves. Figure 6(a) shows the time evolution of the crystal surface morphology, when the two waves are identical. As known from the classical paper of Frank,[24] the bunch gains steps from one side and simultaneously loses steps from the other side. This process is clearly manifested in Figs. 3 and 6. As a result the kinematic wave velocity V_w [the slope of the bunch trajectory in Fig. 3(a)] is lower than the velocity of steps in the core of the bunch. According to Frank V_w is the velocity of an element of the crystal surface with a fixed density of steps and it is instructive to consider V_w as a velocity of the maximum of the step density wave.

To get quantitative knowledge of the dependence of the kinematic wave velocity on the number of steps in the bunch we integrated Eqs. (10) for systems containing different numbers of steps ($10 \leqslant M \leqslant 59$). In all runs the initial conditions were selected to correspond to a configuration with only one bunch, containing almost all steps (just a few steps are outside the bunch). The obtained results are shown in Fig. 7.

The dependence of the kinematic wave velocity on the number of steps in the bunch is an essential factor for the time evolution of the unstable vicinal surface during electromigration affected sublimation. Really, the fast moving small bunches run down the slowly moving large bunches and a dynamic interaction of either the type, shown in Fig. 6(b), or the type shown in Fig. 6(c) takes place. Figure 6(b) manifests rather interesting property of the step density waves, which could be called ''bunch size exchange.'' As seen, when the small bunch approaches the large one, the former starts to increase, whereas the latter decreases by losing steps. The decrease in the number of steps in the initially larger bunch leads to an increase of its kinematic wave velocity. On the contrary, the initially smaller bunch increases and its kinematic wave velocity decreases. As a result the trajectories of the two bunches start to diverge as clearly seen in Fig. 6(b). In Fig. 6(b) the size of the smaller bunch after the dynamic interaction is equal to the size of the smaller bunch before the interaction. It is interesting to note that one could have arrived at the same configuration if the faster step density wave had passed through the slower wave and this process of passing through had caused some retardation of the wave of higher amplitude (in the case of step density waves such a process is impossible for geometrical reasons). The type of dynamic interaction shown in Fig. 6(b) does not affect the size distribution and the average bunch size. It should be noted, however, that deviations from the perfect size exchange occurred very often and the final bunch sizes (after the end of the interaction) were different from the sizes of the initial bunches (in all cases of deviation from the perfect size exchange, however, the final size of the small bunch is smaller than the initial size of the small bunch).

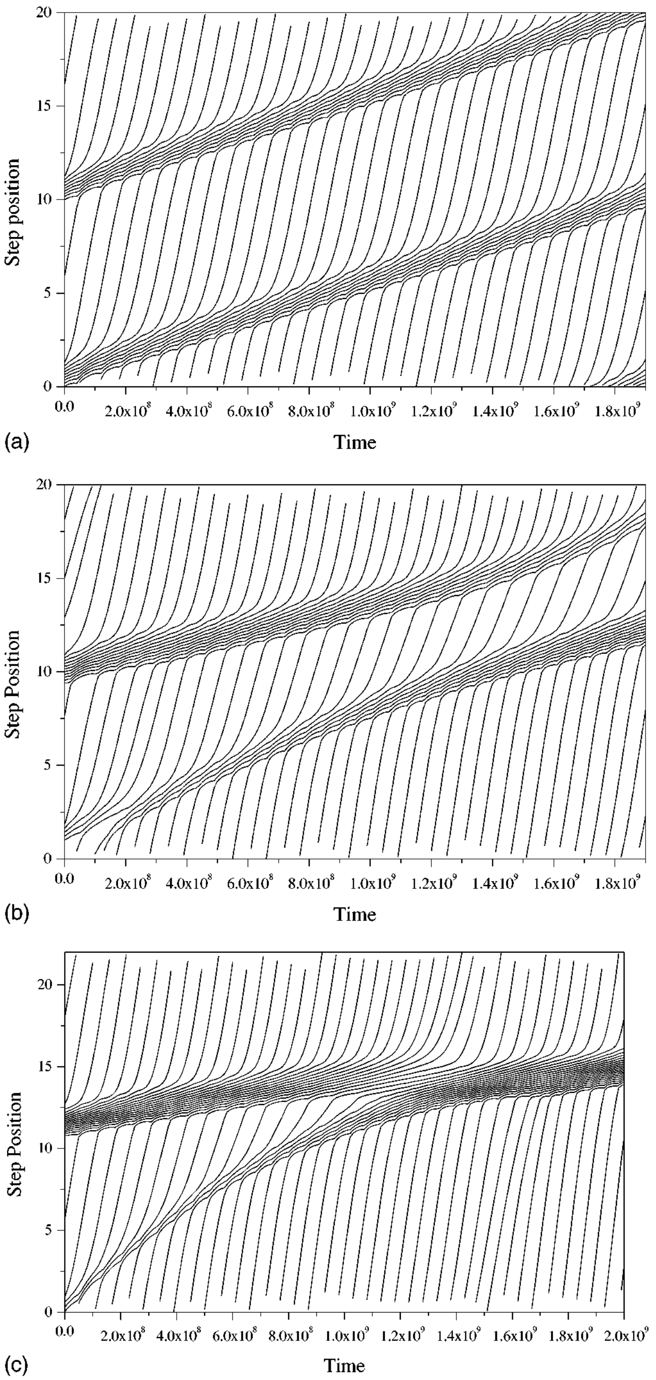

FIG. 6. Trajectories of steps on a crystal surface with two bunches. When the bunches are of equal size (a) they travel at the same velocity and have a steady-state shape. Dynamic interaction of bunches of different size results in either ''bunch size exchange'' (b) or ''effective coalescence'' (c). The parameters in Eq. (10) have the same values as in Fig. 2.

As seen in Fig. 6(c), the second type of dynamic interaction of step density waves is not identical with the process of coalescence, but the result is practically the same (the dynamic interaction of two bunches, containing N_1 and N_2 steps, results in one bunch, containing N_1+N_2 steps). This type of dynamic interaction, which could be called ''effec-

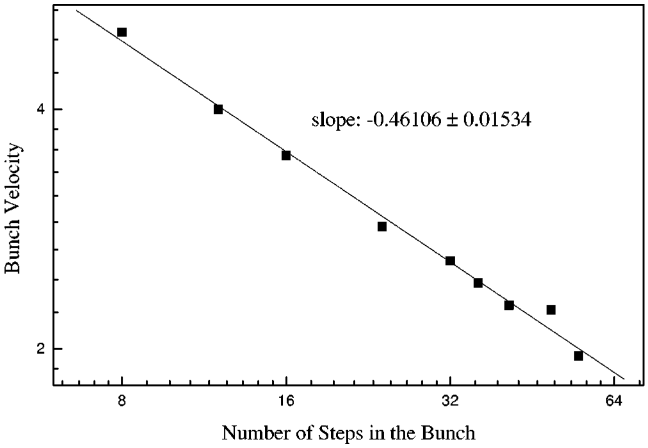

FIG. 7. Kinematic wave velocity as a function of the number of steps in the bunch. These results are obtained by numerical integration of the equations of step motion with the following values of the parameters: $Fl/2kT = -0.000\,06$, $l/\lambda_s = 0.0025$, $\beta\lambda_s/D_s abn_s^e = 117\,000$, and $l_0/l = 0.003$.

tive coalescence,'' provides a ground to revive an old idea of Chernov[16] to consider the time evolution of the crystal surface as a process of coalescence of step density waves. He developed a statistical description of the bunch size distribution (resulting from bunch-bunch coalescence) on the basis of the scaling ideas, formulated by Todes[25] in his analysis of the colloid rapid coagulation (more accessible references on the self-preserving solution of the Smoluchowski equation are the papers of Baroody[26] and Kashchiev[27]). A quantity of considerable importance in the Chernov treatment of bunch-bunch coalescence is the difference $f(N_1,N_2) = V_w(N_1) - V_w(N_2)$ between the kinematic wave velocities of bunches of different size. When the kinematic wave velocity is a homogeneous function of the number of steps in the bunch $[V_w(\eta N) = \eta^{-k} V_w(N)]$ the relative velocity $f(N_1,N_2)$ is also a homogeneous function [it satisfies the relation $f(\eta N_1, \eta N_2) = \eta^{-k} f(N_1,N_2)$] and the average bunch size N_{av} was shown[16] to increase with the sublimation time as $N_{\mathrm{av}} \sim t^{1/(1+k)}$. The results, shown in Fig. 7, produce the value $k = 0.46$ and, therefore, $N_{\mathrm{av}} \sim t^{0.685}$. It is essential to point out, however, that this dependence of the average bunch size on the sublimation time refers to a model, assuming only one type of dynamic interaction of the step density waves — the so-called ''effective coalescence,'' shown in Fig. 6(c). The existence of dynamic interactions of the type ''size exchange,'' shown in Fig. 6(b), is a violation of the basic assumption of the model treated by Chernov. That is why the obtained value 0.685 of the time scaling exponent is not relevant to the time evolution of a morphological instability of vicinal surfaces, where the two types of dynamic interactions between step density waves take place. In fact, this subsection provides mainly qualitative insight of the surface morphology instabilities, caused by electromigration of the adatoms.

IV. RELATION TO THE CONTINUUM MODEL

A continuum equivalent of Eqs. (10) has been obtained by Misbah and Pierre-Louis.[28] They derived a nonlinear equation for the step density and studied the bunching dynamics under different conditions. Here a partial differential equation, corresponding to the set of equations (10) is derived [taking into account the basic relation (7)], and applied to study the steady state shape of a crystal surface having a single bunch of steps. Precisely the same problem, the shape of a bunch between two parallel facets, has been analyzed by Nozieres[32,33] and scaling relations for the width of the bunch have been obtained. The model proposed by Nozieres and the model considered in this paper are different — they contain different physics. The Nozieres model refers to the case of strong correlation between the adatom concentration fields at neighboring terraces, i.e., the adatoms easily cross the steps (in our terminology, the steps are ''transparent'' and the left hand side of Eqs. (7) and (8) is much smaller than the right-hand side). The model analyzed in this paper describes the evaporation kinetics when surface transport, induced by electromigration, is strongly coupled to the exchange between the crystal phase and the adlayer (adatoms rarely cross the steps). Each model could work in one, at least, of the three temperature intervals, where bunching has been observed (at step-down, step-up, and again step-down direction of the heating current). In this way, the transition temperatures (at which the current direction should be reversed to keep the surface unstable to bunching) could reflect a transition from instability, described by the Nozieres model to instability, described by the model, considered in the present paper. It is reasonable to mention that the concentration gradient, assumed in the Nozieres model, could be created by the electromigration force F, pushing the adatoms to the higher facet.

Returning to the continuum model equation for the shape of the crystal surface we could state that it provides an approximate and simplified description of the model. Although one gets some insight in the time evolution of the process, the interpretation of the experimental data should be based on the results obtained from the numerical integration of the set of ordinary differential equations (10). The basis of the derivation is the equation

$$\frac{\partial z}{\partial t} = -h \frac{dx_i/dt}{x_i - x_{i-1}}, \tag{11}$$

where h is the height of a single step and $z(x,t)$ describes the crystal surface shape in the moment t (the $-$ sign on the right hand side accounts for the decrease of z when the steps move in the positive direction of the x axis in Fig. 1). Equation (11) is precisely that used by Frank[24] in developing the kinematic theory of crystal growth and dissolution [$1/(x_i - x_{i-1})$ is the local step density and its product with the rate dx_i/dt of step motion represents what Frank calls step flux]. Substituting Eqs. (10) into Eq. (11) and taking the limit to continuity results in a partial differential equation for $z(x,t)$. For the sake of simplicity one neglects the Schwoebel effect (i.e., one assumes $\beta_u = \beta_d$) and considers a vicinal surface with $\partial z/\partial x > 0$ (see Fig. 1). As far as the equilibrium concentration of adatoms is concerned, it is reasonable to substitute Eq. (4) with the more general expression $n_s^e(x_i) = n_s^e e^{\Delta\mu(x_i)/kT}$, where $\Delta\mu(x_i)$ is the local deviation (due to the curvature) of the chemical potential from the value, characterizing the bulk crystal with a flat surface. Assuming $\Delta\mu(x_i)/kT \ll 1$ and making use of the series expansion of

$\Psi_+(x_i)$, $\Psi_-(x_i)$, $\Phi_+(x_i)$, $\Phi_-(x_i)$ in the case $\alpha(x_i - x_{i-1})/\lambda_s \ll 1$ and $F(x_i - x_{i-1})/2kT \ll 1$ one arrives at the following equation for the time evolution of the crystal surface during heating with a direct current (i.e., in the presence of electromigration of the adatoms):

$$\frac{\partial z}{\partial t} = \frac{D_s n_s^e}{kT}\Omega\left[\frac{\partial^2 \Delta\mu}{\partial x^2} - \frac{F}{kT}\frac{\partial \Delta\mu}{\partial x} + 2F\frac{b}{h}\left(\frac{\partial^2 z}{\partial x^2}\right) + 2F\frac{\partial}{\partial x}\left(\frac{\Delta\mu}{kT}\frac{\partial z}{\partial x}\right)\right] - \alpha^2\Omega\frac{n_s^e}{\tau_s}\left(1+\frac{\Delta\mu}{kT}\right), \tag{12}$$

where $\Omega = abh$ is the atomic volume. The last term in this equation describes the decrease of z due to the desorption flux n_s^e/τ_s of atoms from the crystal surface (the equilibrium concentration of adatoms varies along the surface because of the dependence of the chemical potential on the crystal surface curvature).

In a recent paper Bonzel and Mullins[29] derived the following expression for the local deviation of the chemical potential $\Delta\mu$:

$$\Delta\mu = -\Omega\frac{6\varepsilon \sin\varphi}{\cos^4\varphi}\frac{\partial^2 z}{\partial x^2}, \tag{13}$$

where ε is the same parameter that appears in the expression for the surface free energy:

$$f(s) = f^{(0)} + f^{(1)}s + \varepsilon s^3, \tag{14}$$

with $s = \partial z/\partial x = \tan\varphi$. Equation (13) was derived in a small slope approximation, i.e., the average misorientation angle φ is small, and the local deviation from φ is also small. The latter is not fulfilled in the case of electromigration-induced step bunching, since the maximum slope in a bunch of 16 steps is 10 times larger than the average slope (in the experiments of Williams the minimum interstep distance in a bunch of 16 steps is 124 Å, whereas the average interstep distance determined by the misorientation angle is 1300 Å). Therefore one needs an expression for $\Delta\mu$ with a validity beyond the small slope approximation used by Bonzel and Mullins. Assuming that the step-step repulsion is the only reason for the deviation $\Delta\mu$ of the chemical potential from its value for a bulk crystal with a flat surface one can write

$$\Delta\mu = -\left(\frac{l_0}{x_{i+1}-x_i}\right)^{n+1} + \left(\frac{l_0}{x_i - x_{i-1}}\right)^{n+1} = -\frac{6abA}{h^2}\frac{\partial z}{\partial x}\frac{\partial^2 z}{\partial x^2}, \tag{15}$$

which is valid under the usual assumption $n=2$.

Substituting the last expression into Eq. (12) one arrives at an equation for $z(x,t)$. Here we shall considerably simplify this equation and use it to study the quasiequilibrium shape of a surface profile that connects two infinitely large terraces at different heights, i.e., N elementary steps are situated in the region $0 \leqslant x \leqslant L_b$ and there are no steps at $x<0$ and $x>L_b$. First, we neglect the relatively small terms containing the product of the electromigration force F and the deviation $\Delta\mu$ of the chemical potential from its value at a vicinal surface of zero curvature. Second, we take the limit $\lambda_s \to \infty$, i.e., we consider the shape of the crystal surface in the absence of any desorption. Thus Eq. (12) turns into

$$\frac{\partial z}{\partial t} = \frac{D_s n_s^e}{kT}\Omega\left[-\frac{6abA}{h^2}\frac{\partial^2}{\partial x^2}\left(\frac{\partial z}{\partial x}\frac{\partial^2 z}{\partial x^2}\right) + 2F\frac{b}{h}\left(\frac{\partial^2 z}{\partial x^2}\right)\right]. \tag{16}$$

The quasiequilibrium shape of the crystal surface under consideration will be realized when the step-step repulsion is compensated by the effect of the electromigration inducing force. To determine this shape we consider Eq. (16) as mass conservation law

$$\frac{\partial z}{\partial t} = -\frac{\partial J}{\partial x}, \tag{17}$$

where

$$J = \frac{6abA}{h^2}\frac{\partial}{\partial x}\left(\frac{\partial z}{\partial x}\frac{\partial^2 z}{\partial x^2}\right) - 2F\frac{b}{h}\left(\frac{\partial z}{\partial x}\right). \tag{18}$$

The quasiequilibrium shape $z(x)$ of the crystal surface we define by the requirement that the macroscopic flux of mass be zero, i.e., $J=0$. Thus we arrived at a nonlinear differential equation that has a comparatively simple solution. Really, denoting dz/dx (the quasiequilibrium shape does not depend on time, so that z is a function of only one variable) by y and defining the function $p(y) = (dy/dx)[x(y)]$ one obtains

$$yp\frac{dp}{dy} + p^2 - \frac{F}{A}\frac{h}{3a}y = 0. \tag{19}$$

The substitution $p^2 = \eta$ transforms this equation into

$$\frac{y}{2}\frac{d\eta}{dy} + \eta - \frac{F}{A}\frac{h}{3a}y = 0, \tag{20}$$

which has the solution

$$\eta = \frac{C}{y^2} + \frac{2F}{9A}\frac{h}{a}y, \tag{21}$$

where C is an integration constant. It is reasonable to express the integration constant C through the maximum slope $y_m = (dz/dx)_{\max}$ of the bunch by making use of the condition for an extremum of the function $y(x)$, i.e., $dy/dx = p(y_m) = 0$ and therefore $\eta(y_m) = p^2(y_m) = 0$. On this basis we obtain $C = -2Fhy_m^3/9aA$ and Eq. (21) can be rewritten as

$$\eta = -\frac{2Fh}{9aA}y_m\left[\frac{y_m^2}{y^2} - \frac{y}{y_m}\right]. \tag{22}$$

Since η is positive by definition, the force F should be negative, i.e., the electromigration of adatoms should be in the step-down direction (otherwise the quasiequilibrium shape of the bunch does not exist). Assuming F to be negative one obtains

$$p = \sqrt{\frac{2|F|h}{9aA}y_m}\sqrt{\frac{y_m^2}{y^2} - \frac{y}{y_m}} \tag{23}$$

for the region where the slope (dz/dx) of the crystal surface is an increasing function of x and

$$p=-\sqrt{\frac{2|F|h}{9aA}y_m}\sqrt{\frac{y_m^2}{y^2}-\frac{y}{y_m}} \tag{24}$$

for the part of the crystal surface where the slope (dz/dx) is a decreasing function of x. Since $p(y)= dy/dx$ Eqs. (23) and (24) are easy to integrate differential equations. Thus we arrive at the following equations for the regions of increasing and decreasing slopes correspondingly:

$$\int_0^y \frac{dy}{\sqrt{y_m^2/y^2-y/y_m}}=x\sqrt{2|F|h/9aAy_m}, \tag{25}$$

and

$$-\int_{y_m}^y \frac{dy}{\sqrt{y_m^2/y^2-y/y_m}}=(x-x_m)\sqrt{\frac{2|F|h}{9aA}y_m}, \tag{26}$$

where the values of the integration constants are determined from the conditions $y=0$ at $x=0$ and $y=y_m$ at $x=x_m$. Now we are able to write an expression for the total width L_b of the bunch by making use of the last equations. Since the slope $(dz/dx)=y$ has a value $y=0$ at $x=0$ and $x=L_b$ (in the model under consideration there are no steps at $x<0$ and $x>L_b$) and displays a maximum y_m at $x=x_m$ we can write

$$2\int_0^{y_m} \frac{dy}{\sqrt{y_m^2/y^2-y/y_m}}=L_b\sqrt{\frac{2|F|h}{9aA}y_m}. \tag{27}$$

Introducing a dimensionless variable $\zeta=y/y_m$ results in a more convenient form of the last equation

$$2\int_0^1 \frac{d\zeta}{\sqrt{\zeta^{-2}-\zeta}}=L_b\sqrt{\frac{2|F|h}{9aAy_m}}. \tag{28}$$

Since the left-hand side of the last equation does not contain any physical quantities (the integral in the left-hand side is a dimensionless number), we obtained, in fact, a simple relation between the width L_b of the bunch, its maximum slope y_m, the electromigration inducing force F and the magnitude A of the step-step repulsion. Having in mind that the experimental observations and the results of the numerical integration of the equations of step motion (10) show the average slope Nh/L_b of the bunch to be quite close to the maximum slope y_m, we use the approximation $y_m\approx Nh/L_b$ to rewrite Eq. (28) in the practically more useful (but approximate) form

$$L_b=N^{1/3}\left(\frac{18aA}{|F|}\right)^{1/3}B, \tag{29}$$

where

$$B=\int_0^1 \frac{d\zeta}{\sqrt{\zeta^{-2}-\zeta}}\simeq 0.86.$$

The width L_b of the bunch can be presented as $L_b=(N-1)l_b$, where $l_b$is the average interstep distance inside the bunch. For $N\gg 1$ Eq. (29) can be rewritten as

$$l_b=N^{-2/3}\left(\frac{18aA}{|F|}\right)^{1/3}B. \tag{30}$$

As seen, the average interstep distance in the quasiequilibrium shape of the bunch displays the same scaling exponents (with respect to the number of steps N, the magnitude A of the step-step repulsion, and the electromigration inducing force F) as the minimum interstep distance $l_{\min}$ [calculated by numerical integration of the equations of step motion (10) and shown in Figs. 4 and 5] in a traveling bunch, under the conditions of considerable desorption. It should be pointed out again that Eq. (30) is not an exact result. It is an approximate form of the solution of Eq. (19) [the exact solution is given by Eq. (28)] and, on the other hand Eq. (19) is an approximate form of Eq. (12). Finally, Eq. (30) refers to quasiequilibrium shape of a bunch, whereas the experiments provide data for the steady-state shape. That is why it is not recommendable to use Eq. (30) in the interpretation of results obtained in relevant experiments. The scaling exponents for $l_{\min}$ obtained from numerical integration of the set of equations of step motion are much more reliable. Our numerical results for $l_{\min}$ could be formally presented by an equation identical to Eq. (30) with $B=0.63$ (this value has been extracted from Fig. 4).

It is essential to note that Nozieres[33] obtained a scaling law $l_b\sim N^{-1/2}(A/F)^{1/4}$ for the average interstep distance in a bunch of ‘‘transparent’’ steps. As seen, the Nozieres model, and the model considered in this paper manifest different values of the scaling exponent. This is not surprising because the two models describe different regimes of electromigration affected evaporation of the crystal.

V. CONCLUSION

In the presence of electromigration, the evaporation of a vicinal surface is an interesting combination of two surface processes—mass transport and an exchange between the crystal phase and the adlayer. The mass transport is strongly coupled to the crystal-adlayer exchange when $(\beta/D_sbn_s^e)=1$ (in the terminology of Ref. 7 this is ‘‘kinetics with local adatom conservation’’). In the case of strong coupling the analysis of the mass transport on the crystal surface can be reduced to a diffusion problem on a single terrace. The solution of this problem under relevant boundary conditions provides a ground to derive the explicit form of the equations for step motion in the regime of electromigration affected sublimation. The numerical integration of the equations of step motion reveals that the evaporating crystal surface is unstable (step bunching appears) at the step-down direction of the electromigration inducing force. The quantitative treatment of the electromigration affected sublimation provides a ground to study crystal surface properties like step-step repulsion, surface diffusion, and electromigration.

The central result of this work is the scaling relation $l_{\min}\sim(N^{-2/3})(A/F)^{1/3}$. A striking result of this model is the constant value of $l_{\min}$ in a wide range of values of the average diffusion distance λ_s. Thus one cannot relate the temperature dependence of $l_{\min}$ to the temperature dependence of λ_s. The dependence of $l_{\min}$ on N can easily be determined from relevant experiments and confronted with the last formula to check the validity of the predicted scaling exponent and estimate the value of the ratio A/F.

The scaling relation obtained in this paper provides a remarkable possibility to study the step-step repulsion. The point is that the value of the size scaling exponent depends on the value of n in Eq. (6). We integrated numerically[30] Eqs. (10) assuming $n=1$ and obtained a size scaling relation $l_{\min} \sim N^{-1}$. Therefore the size scaling exponent is a key to the problem of experimentally determining the distance dependence of the step-step repulsion energy.

The different scaling exponents, predicted by the models of ''transparent'' and ''nontransparent'' steps open a new pathway to study the physics of the transition temperatures separating the intervals, where step bunching has been observed at step-up and step-down directions of the electric current. Really, if the size scaling exponents in two neighboring temperature intervals are different, this is an indication for a transition from the Nozieres model[32,33] to the model considered in this paper. If the size scaling exponents are equal, the transition temperature could indicate a change of the sign of the effective electric charge as argued by Kandel and Kaxiras.[21] This conclusion is tempting, but not very reliable. The point is that we obtained the value $-2/3$ for the size scaling exponent of the minimum interstep distance in the bunch, whereas Nozieres obtained[33] a value $-1/2$ for the average interstep distance (in the bunch). In addition, Nozieres analyzed a continuum model, whereas our reliable results were obtained for a discrete model (the motion of each step is followed by integrating the set of ordinary differential equations). Nevertheless, high accuracy experimental data for both minimum and average interstep distances in bunches, containing different number of steps, would elucidate the step-step interaction as well as the mechanisms of the surface processes in crystal evaporation.

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