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LINEAR TENSION OF STEPS AND THERMODYNAMIC STABILITY OF VICINAL SURFACES

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A technique has been developed for determining the linear tension of steps with one-ion and two-ion heights that form growth/evaporation spirals on NaCl(100). This technique is based on the interpretation of experimentally obtained nonlinear dependences of the steady-state distance between spiral's turns in relation to the inverse undersaturation by numerical simulation performed using the analytical solution of the Barton, Cabrera, and Frank diffusion problem, taking into account the step kinetic coefficient and the back stress effect. The linear tension value of steps with one-ion height is found to be less than half the linear tension value of steps with two-ion height. This suggests that the studied vicinal surfaces are thermodynamically stable. The proposed technique can also be applied to other alkali halide crystals.

INTRODUCTION

Understanding the thermodynamic properties of crystal surfaces is essential for comprehending the outcomes of both fundamental and technological studies of these surfaces (see, e.g., [1] and references therein). The linear tension of elementary steps, or the step free energy per unit length, is one of the primary thermodynamic parameters determining surface behavior under conditions of crystal-vapor equilibrium, as well as during growth (evaporation) or other phase transformations [1–4]. In particular, the thermodynamic stability of a given vicinal surface, i.e., its resistance to small perturbations of the surface profile, depends on the nature of the interaction between elementary steps [1, 4, 5]. Monoatomic steps repel each other if their linear tension α_1 is less than half the linear tension α_2 of a double-height step [6]. Such a surface is thermodynamically stable. When $\alpha_2 < 2\alpha_1$, monoatomic steps attract each other, and the surface is thermodynamically unstable.

One applied aspect of studying the dynamics of thermodynamically stable vicinal surfaces under nonequilibrium conditions is the possibility of forming bunches of elementary steps on them, resulting from a "shock in the kinematic wave" [7]. These step bunches on the vicinal surfaces of semiconductor crystals exhibit excellent chemical and electronic properties, which are essential when creating templates for obtaining nanostructures [8, 9].

Previously, we studied the nonlinear dynamics of steps on vicinal surfaces of NaCl(001) in the (100) zone during growth from vapor, leading to the formation of shock waves of the elementary step density [10, 11]. It was shown that in the region of high temperatures and low supersaturation, the kinetic regularities of changes in the step profile of the studied surfaces are characteristic specifically for thermodynamically stable vicinal ones.

This work aimed to determine the linear tension of steps of one- and two-ion heights on NaCl(001) vicinal surfaces and to demonstrate, through the ratio of their values, that the studied surfaces exhibit thermodynamic stability.

ANALYSIS OF APPROACHES

Since the publication of Wulff's classic paper [12], many works have been devoted to the determination of the characteristic energies of a crystal (surface tension, linear tension of steps) as one of the aspects of studying its equilibrium shape (see, for example, [1] and references therein). The approach based on comparing and matching the values of characteristic energies obtained experimentally with calculations performed using density functional theory has provided progress in receiving relevant data for soft metals (see, e.g., [13] and references therein) as well as for some semiconductor crystals (see, e.g., [14]).

For NaCl single crystals, the kinetics of formation and features of the equilibrium pore shape in these crystals were studied in the temperature interval of 690-795 ºC [15]. Using optical and scanning electron microscopy methods, it was shown that all orientations of the $\{hk0\}$ type are represented in an equilibrium shape, and the angular dependences of surface tension γ were found. From the presented dependences, the values $\alpha/\gamma_0 a$ were determined (a is the height of one-ion steps

equal to half the crystal lattice parameter, γ_0 is the surface tension of close-packed faces, according to [16] $\gamma_0 \approx 0{,}3$ J/m^2), which turned out to be equal to 0.64, 0.56, 0.48, respectively, for temperatures of 690, 760 and 795 ºC. The obtained data indicated the thermodynamic stability of vicinal surfaces of the $\{hk0\}$ type in the studied temperature range. At the same time, in such experiments it is always very difficult to draw an unambiguous conclusion regarding vicinal surfaces slightly deviated from the singular face. The difficulty is that experimental research methods do not allow one to reliably establish whether there is a dihedral angle between the singular plane and the nearest vicinal plane in an equilibrium crystal or the transition between them occurs smoothly. If there is a dihedral angle, the orientations within this angle consist of thermodynamically unstable surfaces, and if the transition is smooth, all surfaces are stable.

Estimates of the linear tension of one-ion height steps were made when studying the growth from vapor by the mechanism of random two-dimensional nucleation on the KCl (100) surface [17]. The values of α in the temperature range 315…335 ºC were $6.6 \cdot 10^{-11}$ J/m. This does not contradict the statement about the thermodynamic stability of the vicinal KCl surfaces since $\alpha < \gamma_0 a$, ($\gamma_0 a \approx 9 \cdot 10^{-11}$ J/m), although it is not convincing evidence of thermodynamic stability.

The estimation of the $\alpha/\gamma_0 a$ ratio for NaCl single crystals based on the degree of residual non-isometry of pores in experiments on their shape relaxation under isothermal conditions ($T \cong 730$ ºC) allowed us to obtain a value close to 0.5 [18], which is in agreement with the results of work [15].

A convincing answer to the question about the thermodynamic stability of vicinal surfaces near the singular NaCl(100) can be obtained by determining the linear tensions of steps of one- and two-ion heights. Studies of these surfaces at the microlevel using the well-known electron microscopic technique of vacuum decoration have shown that one of the sources of such steps is screw dislocations with the Burgers vector component normal to the surface. Analyzing the interaction of steps, which form growth/evaporation spirals, with slip bands allows one to measure the step heights [19]. During Langmuir evaporation in the region of low and medium temperatures, spirals having a rounded shape consist of steps of one-ion height $a = 2.81 \cdot 10^{-10}$ m, and faceted spirals are formed by steps of two-ion height $2a$.

In simple phenomenological models of crystalline surfaces, the linear step tension is present in the Gibbs-Thomson relation [20], which is used to express the dependence of the concentration of adatoms in equilibrium with an atomic step on the step curvature [2–4]. In this regard, the step linear tension can play an important role not only in determining the equilibrium configurations of steps but also in controlling their morphological evolution under nonequilibrium conditions.

Thus, by conclusions of the Barton, Cabrera, Frank (BCF) classical theory of layered-spiral crystal growth [2], the critical radius ρ_c of a two-dimensional nucleus depends on the step linear tension α and is related to the distance l between turns of growth spiral by the equation:

$$l = \kappa\rho_c = \frac{\kappa\alpha\omega}{hkT\sigma}, \qquad (1)$$

where ω is the atomic volume; h is the step height; σ is the supersaturation.

Cabrera and Levin calculated the coefficient $\kappa = 19$ for an isotropic growth spiral when the motion of the steps is limited by the rate of adatoms diffusion supply from adjacent terraces (diffusion mode), and the diffusion fields of neighboring steps do not overlap ($\sigma \ll 1$) [21]. Accounting for the decrease in supersaturation in the spiral center at large σ, due to the diffusion removal of adatoms to the first turn (Cabrera and Coleman "back stress effect" [22]), does not lead to a change in the coefficient κ for the diffusion mode.

When the motion of steps is limited by the rate of adatom attachment to them (kinetic mode), spirals take a polygonized shape corresponding to the crystal symmetry. For almost 50 years since the discovery of the dislocation mechanism of crystal growth, various methods for calculating the coefficient κ for polygonized spirals have given a value close to 19 (see, e.g, [23]). Only in the last two decades, after the appearance of several experimental works on the study of the polygonized spiral morphology of some crystals, the validity of the Gibbs-Thomson law use and, in general, the exclusivity of the Kossel crystal model in the crystal growth theory were questioned [24]. Anomalies in the dependence of spiral morphology on supersaturation were observed both during crystal growth from vapor and solution. They were mainly associated with the difference between the growth conditions and the conditions of the local BKF approximation (see [25] and references therein) or with the complexity of the crystal systems under study, to which the developed for Kossel crystals classical concepts (see, e.g., [26, 27]) may not be applicable.

As far as we know, when studying the morphology of growth/evaporation spirals on the NaCl(100) surface, the effects inherent in other types of crystals and required a reconsideration of the validity of using relation (1) were not detected. In particular, they are the Ehrlich-Schwoebel effect, the influence of the dislocation stress field, or the elastic interaction between steps [25]. At the same time, our early studies of the dynamics of one- and two-ion height steps forming growth/evaporation spirals on NaCl(100) showed that the step motion occurs in a diffusion-kinetic mode, although close to diffusion one [28]. This suggested that when studying the dependence of spiral morphology on supersaturation, relation (1) should be revised, taking into account not only the back stress effect [22] but also the finite value of the rate of adatoms attachment to step [29]. The results of numerical spiral modeling based on the expressions obtained in [29] for the radius of the two-dimensional critical nucleus and the velocity of the spiral segment depending on its curvature showed that the distance between the spiral turns depends nonlinearly on the radius of the two-dimensional critical nucleus. The idea of using obtained results to interpret experimental data on the morphology of

growth/evaporation spirals on NaCl(100) at different super-/undersaturation was presented at international conferences (see, e.g., [30]) and is the basis of this work.

EXPERIMENTAL PROCEDURE AND RESULTS

Experimental studies of the dynamics and morphology of one- and two-ion height spiral steps on NaCl(100) surfaces over a wide range of temperatures and undersaturation have been carried out in high-vacuum setup using the electron microscopic technique of vacuum decoration [28]. In one of the installations, it was possible to carry out vacuum cleavages simultaneously of two crystals fixed in independent heaters. By turning the heaters, the cleaved surfaces of the crystals were placed parallelly close to each other. The temperature of the crystals in the heaters was measured using independent thermocouples, and the temperature difference was controlled with a differential thermocouple. Setting a constant temperature difference, evaporation conditions in the range of undersaturation σ from 1 (Langmuir evaporation) to 0.2 were provided on the investigated surface. Lower undersaturation (down to values of ~ 0.01) was created in a setup of a different construction. After heating and vacuum cleavage, the crystals were placed opposite each other in a long cylindrical quartz furnace with a known temperature gradient distribution along its axis. The undersaturation was varied by changing the distance between the crystals.

Systematic studies on the morphology of evaporation spirals at different undersaturations σ were performed at 400 ºC. Fig. 1 shows typical microphotographs of evaporation spirals formed by steps of one- and two-ion heights.

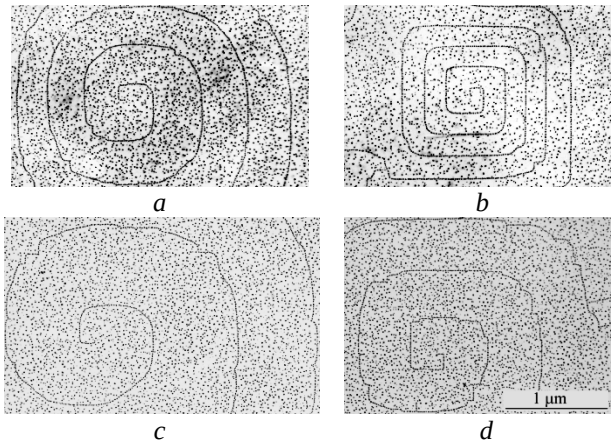

Fig. 1. Typical microphotographs of evaporation spirals formed by steps of one-ion height (a, c) and two-ion height (b, d) at a temperature of 400 °C: $\sigma = 0.25$ (a, b); 0.05 (c); 0.1 (d)

The morphology of spirals was studied at the unsteady evaporation stage when the turns of neighboring spirals do not overlap yet. Such experimental conditions were chosen because, by the velocities of steps, one could reliably control the values of σ measured by the temperature difference ΔT using the known relationship $\sigma \cong \Delta H \Delta T / kT^2$ (ΔH is the evaporation heat) [3]. From photographs of spirals formed over a known time Δt of unsteady evaporation at a given undersaturation σ, step velocities were determined using the relation: $v \approx R/\Delta t$, where R is the radius of the outer spiral turn. Earlier in [28], we obtained a calibration graph of the temperature dependence for the reduced velocity of isolated steps v_{0k}/σ, where k = 1, 2 for one- and two-ion height steps, respectively. Using this graph, taking into account the linear dependence of step velocity on σ known from the theory of elementary crystal growth processes [2, 3], it was possible to reliably control the undersaturation value by measuring step velocities at a given temperature. The linearity of the dependence $v(\sigma)$ was specially checked in control experiments, where for a specific temperature, the values of σ obtained from data on step velocities were compared with σ measured from the temperature difference between the evaporating and growing crystals. Linearity was fulfilled up to approximately $\sigma \approx 5 \cdot 10^{-2}$; at lower values of σ, the uncontrolled impurity presence caused the steps to slow down and deviate from linearity [28].

Since at the non-stationary evaporation stage, the value of l at large σ depends on the distance from the spiral center, i.e., on the terrace number n, the dependences $l(n)$ were plotted for such spirals. The average values $\overline{l_k}$ were determined in the horizontal sections of the corresponding dependences $l(n)$ and were taken equal to the distances between the spiral turns at the stationary evaporation stage.

The obtained values $\overline{l_1}$ and $\overline{l_2}$ for steps of one-ion and two-ion heights, respectively, were plotted as a function of $l(\sigma^{-1})$ (Fig. 2).

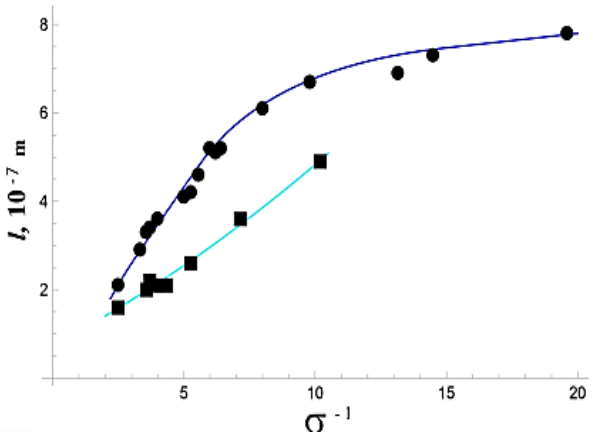

Fig. 2. Graphs of dependence $l(\sigma^{-1})$ for spirals formed by steps of one-ion height (●) and two-ion height (■)

Two features of the presented dependencies are noteworthy. First, the nonlinear character of $l(\sigma^{-1})$, which does not follow from the layered-spiral crystal growth theory [2, 3] (see (1)). Second, for any values of σ, the l_2 values are smaller than l_1. Earlier, $l_2 < l_1$ was observed for the case of Langmuir evaporation in a wide temperature range [31].

If we estimate the values of α_1 and α_2 on the linear sections of the obtained dependences $l(\sigma^{-1})$, it appears that the inequality $\alpha_1 > \alpha_2/2$ takes place. It seems that the NaCl vicinal surfaces are thermodynamically

unstable. But, in addition to this, the values of α_1 turn out to be several times greater than the values of $\gamma_0 a$ and α known from the literature [17]. Such results contradict the data on thermodynamic stability of NaCl(100) vicinal surfaces known from the works, in particular [15, 18].

One of the possible reasons that led to the obtained result may be the difference between the undersaturation in the spiral center and the undersaturation in the vapor phase due to the back stress effect [22]. However, although considering this effect at the value of $\lambda_s \cong 1.31 \cdot 10^{-7}$ m (λ_s is the average diffusion path length of admolecules) for the temperature of experiments [28] leads to a decrease in the values of α_1 and α_2, it does not qualitatively change the relationship between them.

Another reason, in our opinion, is that, as already noted, the motion of spiral steps of one- and two-ion heights occurs in the diffusion-kinetic mode [28]. In [28], the temperature dependences of the surface diffusion coefficients D_s and kinetic coefficients β_{s1} and β_{s2} of steps of one- and two-ion height, respectively, were determined. These data allow one to obtain for a given temperature the values of parameters $Q_1=D_s/\lambda_s\beta_{s1}$ and $Q_2=D_s/\lambda_s\beta_{s2}$, indicating the mode of step motion (at $Q \ll 1$ – diffusion mode, and at $Q \gg 1$ – kinetic). For the temperature of experiments, the corresponding values were: $D_s \cong 8.8 \cdot 10^{-16}$m/s^2, $\beta_{s1} \cong 3.3 \cdot 10^{-7}$m/s, $\beta_{s2} \cong 3.8 \cdot 10^{-8}$ m/s, $Q_1 = 2.04 \cdot 10^{-2}$, $Q_2 = 1.77 \cdot 10^{-1}$.

The fact that the spiral steps move in diffusion-kinetic mode is demonstrated by the change in the morphology of spirals with decreasing undersaturation (see Fig. 1). At high undersaturation, the shape of spirals formed by one-ion steps resemble the equilibrium shape of a two-dimensional nucleus calculated in [2], and the degree of anisotropy decreases from the spiral center to its periphery, reaching a stationary value. With a decrease in undersaturation at a given temperature, the step spacing increases and the shape anisotropy of the peripheral steps decreases.

Spirals formed by steps of two-ion height have faceted shapes at large undersaturation, which was previously associated with the anisotropy of their linear tension [32]. However, Fig. 1 shows that with decreasing σ, i.e., as the system approaches equilibrium, such spirals become rounded. This suggests that the observed shapes are kinetic rather than equilibrium, and their anisotropy is due to the anisotropy of step velocities.

Fig. 1 clearly shows that the anisotropy of the first turn is noticeably expressed concerning the other turns for both types of spirals. The shape of a two-dimensional nucleus growing in the diffusion mode should coincide with its equilibrium shape if the diffusion flows along the steps and over the surface, arising under the action of capillary forces, can ensure a constant value of the chemical potential along the nucleus contour. This is possible if the nucleus has a sufficiently small radius. At increasing radius, when the action of capillary forces related to the nucleus contour curvature can be neglected, the nucleus growing in the diffusion mode should take a rounded shape since the diffusion coefficient on the surface (100) does not depend on the direction. If, however, the nucleus growth occurs in the diffusion-kinetic mode when there is a jump in the chemical potential between the adsorbed phase and the step, the nucleus shape is an anisotropic growth shape, the form of which depends on the anisotropy β_s.

In the processing of experimental data, the results of numerical modeling in [29] were used since there was a qualitative similarity of the experimental dependences $l(\sigma^{-1})$ in Fig. 2 with the dependences of the spiral pitch on the critical nucleus radius obtained earlier for different values of the parameter Q (Fig. 3 in [29]), as well as the diffusion-kinetic mode of step motion and the back stress effect was to be considered. Since the work [29] was not published in English, we introduce below the formulation of the diffusion problem, which was solved in this work, and some main results.

INTERPRETATION OF EXPERIMENTAL RESULTS

To determine the dependence of the velocity of a spiral segment on its curvature radius, it was assumed, as in [22], that the first turn of the spiral with an average effective radius ρ, which most significantly affects the supersaturation in its center, can be replaced with a good approximation by a circle of the same radius. In this case, the diffusion problem is similar to the one discussed in [2, 22] with the only difference: it is necessary to consider the finite rate of adatoms attachment to step.

The surface supersaturation distribution inside (Ψ_1) and outside (Ψ_2) of a two-dimensional nucleus was found from equation [2]:

$$\lambda_s^2 \nabla^2 \Psi(r) = \Psi(r), \Psi(r) = \sigma - \sigma_s(r) \qquad (2)$$

with boundary conditions [3]:

$$\Psi_1(R) = \Psi_2(R),$$
$$\frac{D_s}{\lambda_s}\left[\left.\frac{\partial \Psi_1}{\partial r}\right|_{R-0} - \left.\frac{\partial \Psi_2}{\partial r}\right|_{R+0}\right] = \beta_s[\Psi_R - \Psi_1(R)], \qquad (3)$$

where $R = \rho/\lambda_s$ is the dimensionless radius of a two-dimensional nucleus. All other linear dimensions were also taken in relation to λ_s.

The required values $\Psi_1(r)$ and $\Psi_2(r)$ had the form:

$$\Psi_1(r) = I_0(r)\Psi_R R K_0(R)[Q + R I_0(R) K_0(R)]^{-1},$$
$$\Psi_2(r) = K_0(r)\Psi_R R I_0(R)[Q + R I_0(R) K_0(R)]^{-1}, \qquad (4)$$

where I_0, K_0 is the zero-order Bessel functions of imaginary argument; $\Psi_R = \sigma - \sigma_R$, σ_R is the supersaturation associated with the curvature of a two-dimensional nucleus. At low supersaturations in the vapor phase: $\Psi_R \cong \sigma\left(1 - \frac{R^*}{R}\right)$, where $R^* = \rho^*/\lambda_s$.

Based on (4) and considering the back stress effect and parameter Q, an expression for the dimensionless radius of a two-dimensional critical nucleus R_s^* was found. After substituting Ψ_R and $\Psi(R) = \Psi_1(R) = \Psi_2(R)$ into (3), an expression was obtained for the dependence of spiral segment velocity on its curvature radius $v(R)$, which was used for numerical simulation

of the process of polygonized (square) spiral formation [29].

By varying the values of R^* and Q as parameters, it was shown that the proportionality coefficient between the spiral pitch L and radius of a two-dimensional critical nucleus (R^*, and also, R_s^*) is not a constant value. Since the parameter Q characterizes the ratio of the rate of diffusion supply of adatoms to the step ($\sim D_s/\lambda_s$) to the rate of adatom attachment to the step ($\sim\beta_s$), an important conclusion concerning the morphology of spirals follows from the obtained result: steps of various heights with different kinetic coefficients form spirals with different pitches at the same effective surface tension of the step face (α/h).

This conclusion qualitatively explains the difference, presented in Fig. 2, in the distance between the turns of spirals formed by steps of different heights at the same undersaturation. As shown above, the kinetic coefficients of the one-ion height steps β_{s1} are almost an order of magnitude greater than those of the two-ion height steps β_{s2}.

For quantitative processing of experimental data, the dependences of $\overline{l_1}$ and $\overline{l_2}$ divided by λ_s on σ^{-1} were plotted. Using the obtained values of L as a parameter and comparing experimental dependences $L(\sigma^{-1})$ with calculated $L(R^*)$ for the obtained values of parameters Q_1 and Q_2, the corresponding values of the dimensionless radii for critical two-dimensional nuclei R^* were found. The obtained dependences $R^*(\sigma^{-1})$ for spirals formed by steps of one-ion (1) and two-ion (2) heights are presented in Fig. 3. From the slope of obtained straight lines and using relation (5),

$$R^* = \frac{\alpha\omega}{h\lambda_s kT\sigma}, \qquad (5)$$

the values of linear tension α_1 and α_2 for one- and two-ion height steps, respectively, were found:

$$\begin{aligned} \alpha_1 &= (29.3 \pm 3.1)\ \text{meV/Å}, \\ \alpha_2 &= (106.1 \pm 12.5)\ \text{meV/Å}. \end{aligned} \qquad (6)$$

Comparison of α_1 with the value obtained for one-ion height steps on the (100) KCl surface in [17] gives good agreement. In addition, the value of the ratio $\alpha_1/\gamma_0 a$ agrees with the values obtained in [15, 18].

The determined values of α_1 and α_2 satisfy the inequality $\alpha_1 < \alpha_2/2$, indicating the existence of repulsive forces between elementary steps and, thus, the thermodynamic stability of the NaCl(100) vicinal surfaces.

This can be confirmed by the experimentally observed fact that at low undersaturation, i.e., under conditions close to the thermodynamic equilibrium state, the splitting of steps of two-ion height into steps of one-ion height occurs (Fig. 4). The splitting of double steps is caused by the decreasing influence of kinetic factors on their stability, and it is the manifestation of repulsive forces of a thermodynamic nature between elementary steps.

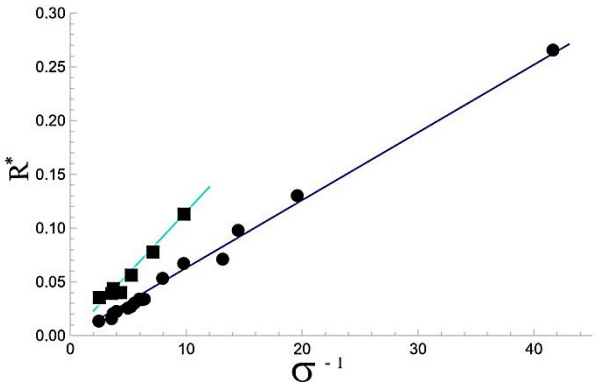

Fig. 3. Graphs of dependence $R^*(\sigma^{-1})$ for spirals formed by steps of one-ion height (●) and two-ion height (■)

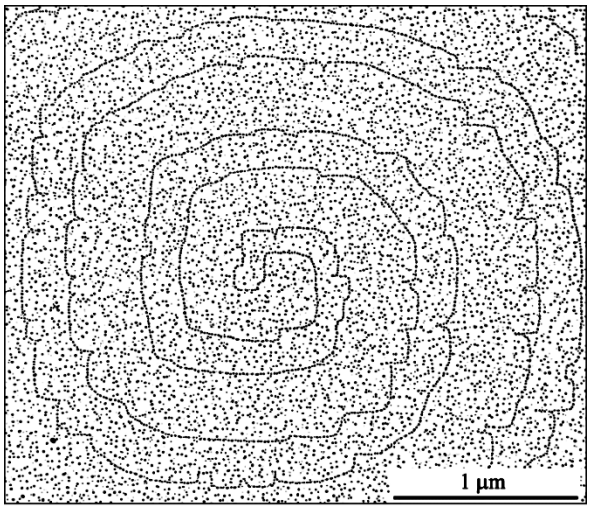

Fig. 4. Splitting of a spiral step of two-ion height into two steps of one-ion height in the region of small undersaturations at temperature 400 °C: σ =0.05

CONCLUSIONS

Within the range of undersaturation, spanning from 1 (Langmuir evaporation) to 0.02 at a temperature of 400 °C, it was analyzed the electron microscopic images of spiral steps formed around the points where screw dislocations, having a normal component of the Burgers vector equal to half or an integer crystal lattice parameter, emerge on the NaCl(100) surface. The morphology of these spirals is discussed, and it is shown that the anisotropy of spiral turns at the same distance from their center decreases with decreasing undersaturation. This suggests that the observed anisotropic shapes of the spirals are not thermodynamic but kinetic. In other words, the anisotropy in the shape of spiral steps is not related to the anisotropy of their linear tension, as previously believed. Instead, it is due to kinetic factors, including (i) the diffusion-kinetic mode of the motion of a spiral step, when the anisotropic shape of a two-dimensional nucleus growth depends on the anisotropy of the kinetic coefficient of the step, and (ii) the back stress effect, which leads to a decrease in undersaturation in the spiral center due to the overlap of diffusion fields of the central spiral turns.

Systematic measurements of the steady-state distances between the turns of spirals formed by one-ion and two-ion height steps (l_1 and l_2, respectively) as a function of the inverse undersaturation (σ^{-1}) were performed. It is shown that dependences $l(\sigma^{-1})$ are nonlinear, which contradicts the conclusions of the theory of layered-spiral crystal growth from vapor in the diffusion mode of step motion. Furthermore, not only in the case of Langmuir evaporation (well-known from the papers) but also across the entire range of investigated undersaturation, the values of l_2 turned out to be less than l_1. Estimates of the linear tension values of one- and two-ion height steps (α_1 and α_2, respectively) based on existing theoretical concepts revealed that α_1 exceeds the known data by several times, and the obtained ratio $\alpha_1 > \alpha_2/2$ contradicts the ideas regarding the thermodynamic stability of vicinal surfaces of alkali-halide crystals.

The revealed features in spiral pitch change with decreasing undersaturation qualitatively agree with the results of numerical simulation conducted using the analytical solution of the Barton, Cabrera, Frank diffusion problem, while considering the finite value of the kinetic coefficient of steps and the back stress effect. Using these results for parameters corresponding to the experimental conditions allowed us to rearrange the experimental dependences $l(\sigma^{-1})$ in the coordinates $R^*(\sigma^{-1})$, where R^* is the radius of the two-dimensional critical nucleus, normalized by the average diffusion path length of admolecules. The linearity of the obtained dependences, by the straight line slopes, enables the determination of the linear tension of one- and two-ion height steps: $\alpha_1 = (29.3 \pm 3.1)$ meV/Å, $\alpha_2 = (106.1 \pm 12.5)$ meV/Å.

The fact that the value of α_1 is less than half the value of α_2 indicates the presence of repulsive forces between elementary steps, suggesting the thermodynamic stability of NaCl(100) vicinal surfaces. An indirect confirmation of this stability is the experimentally observed splitting of two-ion height spiral steps into two spiral steps of one-ion height at low undersaturation.

Given the consistency of the obtained value of α_1 with the value known for potassium chloride crystals from the references, the developed methodology for determining the linear tension of steps can be applied to other alkali-halide crystals.

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ЛІНІЙНИЙ НАТЯГ СХОДИН І ТЕРМОДИНАМІЧНА СТАБІЛЬНІСТЬ ВІЦИНАЛЬНИХ ПОВЕРХОНЬ

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Розвинена методика визначення лінійного натягу сходин одноіонної та двохіонної висоти, що утворюють спіралі росту/випаровування на поверхні NaCl(100). Методика заснована на інтерпретації експериментально отриманих нелінійних залежностей встановленої відстані між витками спіралі від зворотного недосичення шляхом чисельного моделювання з використанням аналітичного розв'язку дифузійної задачі Бартона, Кабрери та Франка з урахуванням кінетичного коефіцієнта сходини та ефекту зворотного впливу. Значення лінійного натягу сходини одноіонної висоти виявилося менше половинного значення лінійного натягу сходини двохіонної висоти. З цього випливає, що досліджені віцинальні поверхні термодинамічно стабільні. Запропонована методика може бути використана для інших лужно-галоїдних кристалів.