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VERIFICATION OF ONE-DIMENSIONAL MODELS DESCRIBING ANISOTROPY OF STEP GROWTH

Models that allow to obtain directional dependencies of normal velocity of a straight step on the (001) face of Kossel crystal and its edge free energy are reviewed. The dependencies were considered in a wide range of crystal growth conditions, which showed some significant discrepancies between the models and limitations in the scope of their applicability. The results presented concern on one-dimensional kinetic and thermodynamic models of a single step.

Keywords: step growth, Burton Cabrera Frank theory, Monte Carlo simulation of crystal growth.

1. INTRODUCTION

The growth of a perfect crystal is possible only when nuclei of critical size are forming on its surface. However, the rate of creation of critical nuclei, which can be estimated on thermodynamical basis, is too small to explain many experimental data on the growth rate. This observation led Frank to formulate suggestions that those crystals which grow are not perfect and the steps on the crystal surface are generated by dislocations [1]. Therefore, a need arose to develop theoretical models predicting the structure of the step, its edge free energy, velocity of motion and their directional dependencies. Among the published works, the theory developed by Burton, Cabrera and Frank (BCF) in 1959 [2] is particularly well known and is still cited in recent papers. While the BCF theory is based on thermodynamic grounds, a kinetic approach has been applied in some other works. The latter include mainly analytical approach based on a stationary kinetic equation method [3-5] and some fragmentary results obtained using of one-dimensional (1D) Monte Carlo (MC) simulations [6] and two-dimensional (2D) MC simulations [7-9]. Although many other works on crystal growth are known from the literature, most of them do not provide any quantitative description of anisotropy of step growth.

The motion and interaction of the spirals generated by different dislocations significantly affect the kinetics of crystal growth. However, available quantitative analyzes of this effect are still focused on a particularly simple case of isotropic spirals [10-14]. In the anisotropic case, an equation describing time evolution of any contour may be formulated as in Ref. [15] based on the Ginzburg-Landau theory

$$\frac{\partial \xi}{\partial t} = -D(\theta)\left[\left(\gamma(\theta) + \frac{d^2\gamma}{d\theta^2}\right)\frac{1}{R} - \Omega^{-1}\Delta\mu\right],$$ (1)

where ξ is the local displacement of the contour in the normal direction **n**, D is a transport coefficient, θ is the angle between **n** and any fixed vector in the system, R is the local radius of curvature of the contour, Ω is the area covered by a single growth unit, and $\gamma \Omega^{1/2} = F$ is the edge free energy per unit length of the contour. As can be seen from Eq. (1) the coefficient D is proportional to the normal velocity V of straight step. In the isotropic case Eq. (1) reduces to the form known the BCF theory $d\xi/dt = V(1 - R_c/R)$, where R_c is the critical radius. For the anisotropic motion, the directional dependencies $D(\theta)$ and $F(\theta)$ must be known from other models.

The aim of this work is to review the directional dependencies $D(\theta)$ and $F(\theta)$ resulting from models known from the literature, critical analysis of results obtained in a wide range of parameters characterizing crystal growth conditions and drawing some conclusions. Due to the wide range of necessary analyzes, we will focus in this work on 1D models. Although the 1D one-dimensional approach is relatively old, it still remains the only one for which a completely analytic derivation of the $D(\theta)$ and $F(\theta)$ dependencies is known from literature.

2. THEORY

All the works that concern one-dimensional models use some common assumptions to simplify description of a microscopic state of a step. First of all, only the (001) face of Kossel crystal is considered. Moreover, the assumption known as "solid-on-solid" is applied for two perpendicular crystallographic directions, which allows one to describe the state of a step by 1D array $h(x)$ containing the heights of columns of solid blocks in monoatomic layer (Fig. 1). This restriction excludes overhangs in a step, and limits all possible processes to locations lying on the edge of the step. The difference of columns heights at the two neighbouring locations $h(x + 1) - h(x)$ determines the height of kink k, which may take any integer values $0, \pm1, \pm2,...$ measured in lattice constant units.
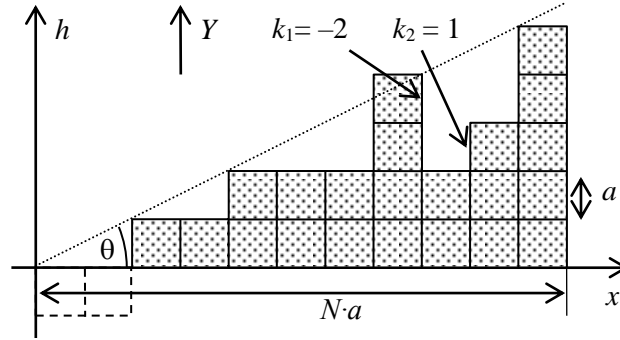
Fig. 1. The growth step on the (001) face of Kossel crystal considered as a columns of solid blocks in monoatomic layers

Let $X(k)$ be the probability of finding a kink of height k. The probability of finding any kink is

$$\sum_{k=-\infty}^{+\infty} X(k) = 1.$$ (2)

Following the works [2,5], the average orientation of the step will be described by the parameter h

$$h = \tan\theta = <k> = \sum_{k=-\infty}^{+\infty} k\, X(k).$$ (3)

where θ is the angle between the step and the $+x$ crystallographic axis (Fig. 1).

Correlation between kinks at neighbouring locations leads to a system of equations, which has not been solved analytically. Therefore, the correlation was neglected in analytical works, including both the BCF theory and the works based on kinetic equations. Hence, the approximate value of the probability $X(k_1, k_2, \ldots)$ of finding a given combination of neighbouring kinks [2, 4, 5] is

$$X(k_1, k_2, \ldots) \approx X(k_1) X(k_2) \ldots .$$ (4)

The correlation may be, however, examined by MC simulations.

Further derivations of probabilities $X(k)$ are different in the BCF theory and in the approach based on kinetic equation.

2.1. BCF model

The paper publisher by Burton, Cabrera and Frank [2] refers to a number of 2D and 3D concepts, such as two-dimensional nucleation and growth pyramids. In this work, however, we refer only to that part of the paper where the problem of the structure of a step is a 1D problem.

In the BCF theory, particular processes between some selected configurations of kinks in equilibrium have been considered (a detailed description of the processes taken into account can be found in Appendix C of Ref. [2]). If the energies of the two configurations are the same, the probabilities of their occurrence are equal $X(k_1, k_2, \ldots) = X(k'_1, k'_2, \ldots)$. When the energy ϕ_{SS} of solid nearest neighbours interaction must be supplied in going from $(k_1, k_2, \ldots)$ to $(k'_1, k'_2, \ldots)$ configuration, the probabilities satisfy the following relationship

$$X(k'_1, k'_2, \ldots) = X(k_1, k_2, \ldots)\eta^2. \tag{5}$$

The term η in Eq. (5) is defined as

$$\eta = \exp(-\phi_{SS}/2k_B T), \tag{6a}$$

where k_B is the Boltzmann constant and T is temperature. In the original formulation of the BCF theory, only the energy ϕ_{SS} of solid-solid bonds is taken into account. Following thermodynamic models of Jackson [16,17] and Temkin [18] as well as kinetic models [5,6,19-21], we will also include the energies ϕ_{FF} and ϕ_{SF} of fluid-fluid and solid-fluid bonds. Each process considered in BCF, which leads to a change in the configuration of atoms without changing the number of atoms forming a crystal, is associated with a change in the energy by a certain multiple of factor $\alpha/2$. Equation (6a) can therefore be generalized as

$$\eta = \exp(-\alpha/4), \tag{6b}$$

where α is the Jackson-Temkin parameter

$$\alpha = (2\phi_{SS} + 2\phi_{FF} - 4\phi_{SF})/k_B T. \tag{7}$$

It can be proved from equations (2)-(5) that the following relations must be satisfied [2]

$$X(k) = \begin{cases} X(0)g_-^{-k}, & \text{for } k < 0, \\ X(0)g_+^{k}, & \text{for } k \geq 0, \end{cases} \tag{8}$$

where $0 \leq g_\pm \leq 1$ and

$$g_+ g_- = \eta^2, \tag{9}$$

$$X(0) = \left[1 + \eta^2 - \sqrt{\left(1 + \eta^2\right)^2 - \left(1 - \eta^2\right)^2\left(1 - h^2\right)}\right] \bigg/ \left(1 - \eta^2\right)\left(1 - h^2\right), \tag{10}$$

$$2g_+ = 1 + \eta^2 - X(0)(1 - \eta^2)(1 - h), \tag{11}$$

$$2g_- = 1 + \eta^2 - X(0)(1 - \eta^2)(1 + h). \tag{12}$$

The dependence of the normal velocity of a straight step on its direction $V(h)$ has not been proposed in the original formulation of the BCF model. Following the argumentation presented *e.g.* in Refs. [15, 22], crystal growth

occurs primarily by the absorption of atoms at kinks. Consequently, the transport coefficient D and the normal velocity V are proportional to the density of kinks C

$$D(h) \sim V(h) \sim C = [1 - X(0)](1 + h^2)^{-1/2}, \tag{13}$$

where $[1 - X(0)]$ is the density along the [1,0,0] direction and the term $(1 + h^2)^{-1/2} = \cos\theta$ allows to obtain the density per unit length of the step.

In the BCF theory the configurational free energy per unit length of a straight step was found as $F = (U - TS)(1 + h^2)^{-1/2}/N$. The internal energy of the step is $U = (N + \Delta N_{SF})\alpha k_B T/4$, where $N\alpha k_B T/4$ is the energy of a perfectly straight step and $\Delta N_{SF} = N \sum_{k=-\infty}^{+\infty} |k| X(k)$ is the increase in the number of solid-fluid bonds due to the formation of kinks. The entropy S is given by the Boltzmann formula $S = k_B \ln W$, where W is the number of ways in which $[1 - X(0)]N$ kinks of any height can be arranged in N locations. In this calculation $X(k)N$ kinks of a given height k are treated as undistinguishable, while the kinks of different heights are distinguishable. This reasoning together with equations (2), (3) and (8) allows us to derive the formula

$$
F = k_B T \left\{ \left[1 + \frac{X(0)g_-}{(1 - g_-)^2} + \frac{X(0)g_+}{(1 - g_+)^2} \right] \frac{\alpha}{4} + \right.
$$
$$
\left. + \left[\ln X(0) + \frac{X(0)\, g_- \ln(g_+ g_-)}{(1 - g_-)^2} + h \ln g_+ \right] \right\} (1 + h^2)^{-1/2}. \tag{14}
$$

The approach based on the kinetic equation (which is discussed is section 2.2) may lead to other values of $(g_+ g_-)$, $X(0)$, g_+, g_- than those given by Eqs. (9)-(12) but the formula (14) still remains correct. In the particular case when the solution (9) can also be used, the formula (14) simplifies to the form known from the original formulation of the BCF theory [2]

$$F = k_B T \left\{ (1 + h)\alpha/4 + \left[\ln X(0) + h \ln g_+ \right] \right\} (1 + h^2)^{-1/2}. \tag{15}$$

2.2. Kinetic analytical approach

In the kinetic approach, the rates $dX(k)/dt$ are associated with fluxes of molecules being created and annihilated at the edge of the step. In particular, where diffusional processes are neglected and approximation (4) is applied we get the following equality for a stationary state [5]

$$\frac{dX(k)}{dt} = U_R(k+1)X(k+1) + V_R(k-1)X(k-1) - [U_R(k) + V_R(k)]X(k) = 0, \tag{16}$$

where

$$U_R(k) = \sum_{k_1=-\infty}^{+\infty}[\nu^+(k_1,k)+\nu^-(k,k_1)]X(k_1), \tag{17}$$

$$V_R(k) = \sum_{k_1=-\infty}^{+\infty}[\nu^+(k,k_1)+\nu^-(k_1,k)]X(k_1), \tag{18}$$

and $\nu^+(k_1, k_2)$ and $\nu^-(k_1, k_2)$ are the frequencies of creation and annihilation, respectively, at a column between a kink of height k_1 on the left and k_2 on the right. The stationary normal velocity of the step is given by

$$V = a\cos\theta \sum_{k_1,k_2=-\infty}^{\infty}\left[\nu^+(k_1,k_2)-\nu^-(k_1,k_2)\right]X(k_1)X(k_2), \tag{19}$$

where a is the lattice constant.

If ν^+ and ν^- depend only on the signs of k_1 and k_2 (negative, zero or positive), but do not depend on the height of a kink, the exact solution of Eq. (16) is again in the form (8). Moreover, taking advantage of Eqs. (2), (3) and (8) one can express $\delta = g_+ + g_-$ as a function of $\kappa = g_+g_-$ and of the average step orientation h [5]

$$\delta = \left[\sqrt{h^2(1-\kappa)^2+4\kappa} - h^2(1+\kappa)\right]/(1-h^2). \tag{20}$$

The value of κ appear to depend on the choice of the ν^+ and ν^- frequencies. There are two different types of dynamics known from classic works on 2D MC simulations [19-24] which were later adapted to 1D simulations [6] and 1D analytical models [5]:

A) In the case of growth from vapour, no energy barrier exists for attaching the atom to the crystal and the frequency of creation does not depend on the local configuration of neighbouring atoms

$$\nu^+ = f_t e^{\beta-\gamma}, \quad \nu_i^- = \nu^+ \exp[\alpha(2-i)/2-\beta]. \tag{21}$$

B) If the free energy of activation of viscous flow in the mother phase is very important then the rates are symmetric

$$\nu_i^+ = f_t \exp[-\alpha(2-i)/4+\beta/2], \quad \nu_i^- = f_t \exp[\alpha(2-i)/4-\beta/2]. \tag{22}$$

In equations (21) and (22) f_t denotes a constant factor with a dimension of frequency, i is the number of nearest solid neighbours, and the conditions of crystal growth are given by Jackson-Temkin parameter α defined by Eq. (7) and the second parameter

$$\beta = (\mu_f - \mu_s)/k_B T, \tag{23}$$

where μ_f and μ_s are the chemical potentials of fluid and solid particles. In the case of 2D models, the number $i = 0, 1, 2, 3,$ or 4 when the neighbour in the

previous completely solid layer is omitted. The second SOS assumption made in 1D models limits the possible values to:

$$i(k_1, k_2) = \begin{cases} 1 & \text{for } k_1 > 0 \text{ and } k_2 < 0, \\ 2 & \text{for } (k_1 > 0 \text{ and } k_2 \geq 0) \quad \text{or} \quad (k_1 \leq 0 \text{ and } k_2 < 0), \\ 3 & \text{for } k_1 \leq 0 \text{ and } k_2 \geq 0. \end{cases} \tag{24}$$

The use of dynamics (21) in the kinetic equation (16) leads to

$$\kappa = \frac{e^\beta + e^{-\alpha/2}}{e^\beta + e^{\alpha/2}}. \tag{25}$$

Here we have corrected an editorial error in the formula (25) that was previously made in Ref. [5], while the other formulae and plots seem to be correct. The dynamics (21) together with Eqs. (2), (8) and (19) allow to determine the following normal velocity of the step [5]

$$V = f_t a \cos(\theta) e^{-\alpha} \left[e^\beta - \frac{\left(e^{\alpha/2} \kappa + e^{-\alpha/2} \right)(1 - \delta + \kappa) + \delta - 4\kappa + \kappa\delta}{(1 - \kappa)^2} \right]. \tag{26}$$

The dynamics (22) substituted into the kinetic equation (16) leads to [5]

$$\kappa = e^{-\alpha/2}, \tag{27}$$

which means that the structure of the step is always the same as in equilibrium state ($\beta = 0$). The velocity (19) for the dynamics (22) takes the form [5]

$$V = 2 f_t a \cos(\theta) \sinh(\beta/2) \frac{2 e^{-\alpha/4} + \delta}{\left(1 + e^{-\alpha/4} \right)^2}. \tag{28}$$

The edge free energy has not been considered in works [3-6] employing the 1D kinetic approach but the formula (14) resulting from the BCF theory may always be applied together with the results of kinetic analytical approach. Unfortunately, it is difficult to indicate any method suitable for MC simulation, where the lack of correlation between neighbouring kinks may not be assumed.

2.3. Kinetic one-dimensional Monte Carlo simulations

In 1D MC simulations the current state of solid-fluid interface is described by the array $h(x)$ stored in computer memory and updated after each random event. Therefore, the frequency of creation and annihilation are always unambiguously known for every possible location x, and the probabilities X together with the approximations (4) and (8) are no longer needed. In order to obtain the assumed step orientation θ, the ends of the array $h(0)$ and $h(N-1)$ are connected cyclically with an additional shift in the direction of the Y axis. The normal velocity of the step results directly from the increase ΔN in the number of atoms in the crystal at the time Δt [6, 21]

$$V(\theta) = \frac{a\,\Delta N\cos\theta}{N\,\Delta t}\,; \quad \Delta t = \sum_j \tau_j\,; \quad \tau_j = \sum_{i=1}^{3}\left(n_{ij}^{\mathrm{F}}\nu_i^{+} - n_{ij}^{\mathrm{S}}\nu_i^{-}\right), \qquad (29)$$

where τ_j is the time passing between the *j*-th and the next elementary event, and n_{ij}^{F} and n_{ij}^{S} are numbers of fluid and solid blocks at the interface, respectively, surrounded by *i* solid lateral neighbours after the *j*-th event.

The algorithm of MC simulations of crystal growth described by Gilmer and Bennema in Ref. [19] is one of the simplest to implement, but also one of the least effective, especially for high values of the α parameter. In this work, we use an algorithm, which is a 1D version of the quick algorithm described in Ref. [21]. The choice of the algorithm, however, should affect only the time necessary to complete the simulation but not the results of simulations.

3. RESULTS AND DISCUSSION

This is known from 2D MC simulations that the layer-by-layer growth mechanism manifests itself on the (001) face of Kossel crystal when $\alpha > 3.2 \dots 3.5$ [25]. According to our best knowledge, the predictions resulting from 1D models described in section 2 have not been analyzed before for such small values of α. In addition, only the plots of the growth velocity ($V/\cos\theta$) in column direction *Y* (see Fig. 1) have been presented in previous papers on the kinetic approach (see *e.g.* [5, 6]), which makes it difficult to assess the normal velocity *V*. The $V(\theta)$ and $F(\theta)$ dependencies given by the formulas (13) and (15) resulting from the BCF theory have been used to plot some spirals growing around screw dislocations (see, *e.g.* Ref. [15]). However, the plots of these dependencies probably have not been presented and discussed anywhere.

3.1. BCF model

The dependencies derived in Chapter 2 on the basis of 1D description of the step, apply directly only to the orientations $0° \leq \theta \leq 45°$ [2,15]. The use of these dependencies for any step may therefore require additional relationships resulting from the symmetry of assumed (001) face of Kossel crystal, such as *e.g.* $V(-\theta) = V(\theta)$ and $V(45° - \theta) = V(45° + \theta)$. However, as can be seen in Figs. 2, 4 and 5, the functions $V(\theta)$, $F(\theta)$, $\mathrm{d}^2F(\theta)/\mathrm{d}\theta^2$ appearing in Eq. (1) are not smooth in the extended range of θ and the results obtained for $\theta = 45° + n\,90°$ should be considered as non-physical. Unfortunately, we cannot even say that the functions are nearly smooth with some good approximation for layer-by-layer growth mechanism when $\alpha \in 3.5 \dots 8$.
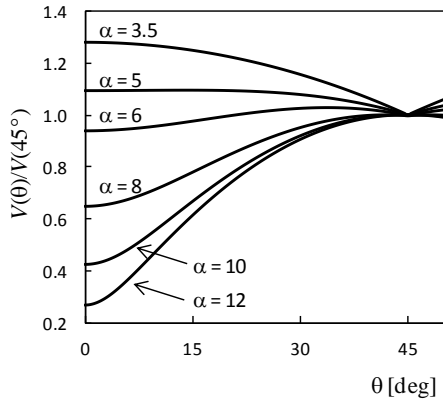
Fig. 2. Normal velocity of a step V given by Eq. (13) as a function of the step azimuth θ normalized to the level of velocity for $\theta = 45°$
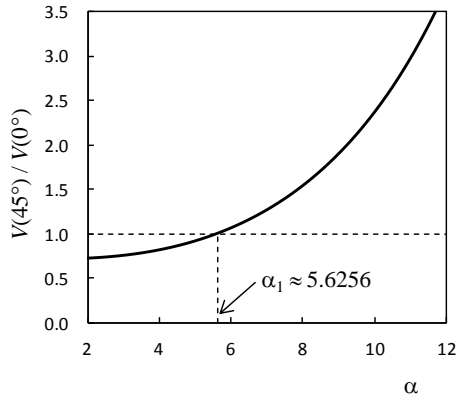

Fig. 3. Ratio of normal velocities V given by Eq. (13) for $\theta = 45°$ and $\theta = 0°$ as a function of the α parameter
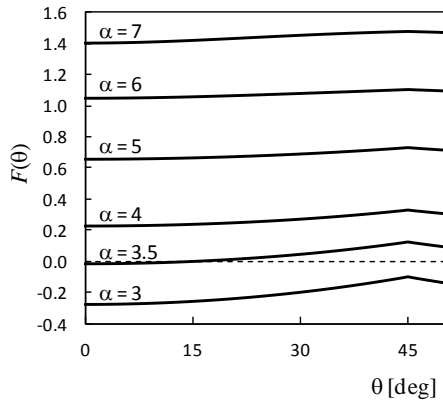

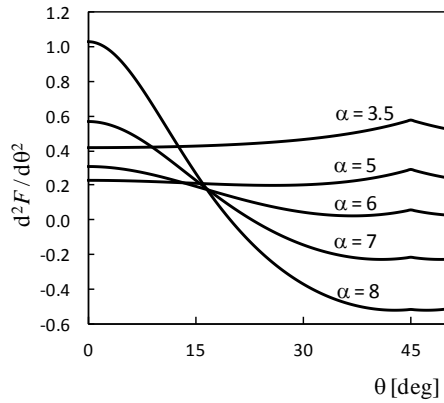Fig. 4. Edge free energy F per unit length of a step given by Eq. (15) as a function of the azimuth θ of its orientation

Fig. 5. The second derivative of edge free energy F per unit length of a step with respect to the azimuth θ of its orientation as a function of θ. $F(\theta)$ is given by Eq. (15)

The minimum and maximum of the $V(\theta)$ dependence can be expected for $\theta = 0°$ and $\theta = 45°$ [7-9, 15]. The ratio of normal velocities $V(45°)/V(0°)$ is therefore useful as a measure of the anisotropy of normal velocity. It can be seen in Fig. 3 that all three relations $V(45°) > V(0°)$, $V(45°) = V(0°)$ and $V(45°) < V(0°)$ are possible for V calculated according to Eq. (13). Because the boundary value $\alpha_1 \approx 5.6256$ for $V(45°) = V(0°)$ is in the area of the layer-by-layer growth mechanism, three qualitatively different cases could be expected in 2D models of spiral growth, namely: isotropic spiral and polygonized spirals with two possible orientations relative to the crystallographic axes. However, this prediction does not agree with the results of 2D MC simulations (see, e.g., Refs. [7, 9]).

3.2. Kinetic analytical approach

When the frequencies of elementary events are given by the formula (22), the kinetic approach and the BCF theory lead to the same state of the step $X(k)$ given by Eq. (8), where the g_+ and g_- factors are determined by equivalent equations (20) and (27) for the kinetic approach or (6b), (9)-(12) in the case of the BCF theory. It should be noted, however, that in the BCF theory the values of $X(k)$ were found only for equilibrium state $\beta = 0$, while in the kinetic model any value of β was allowed and the lack of dependence of $X(k)$ on β was proved.

The normal velocities $V(\theta)$ calculated according to the formula (28) from the kinetic analytical model and shown in Figs. 6 and 7 differ significantly from the velocities in Figs. 2 and 3 resulting from the formula (13). Because we compare here the velocities corresponding to the same dynamics (22) and the same state $X(k)$, the only source of observed differences lies in the two methods used to calculate the velocity. Certainly the formula (28), which takes into account various configurations of neighbouring atoms, should be considered as more accurate than the formula (13) based on total number of any kinks.

The frequencies of elementary events given by the formula (21) lead to the solution (25) and the normal velocity (26). As it can be seen in Figs. 8 and 9, the velocity is noticeably different from that in Figs. 6 and 7 corresponding to the dynamics (22). Derivation of probabilities $X(k)$ equivalent to the dynamics (21) does not seem possible on the basis of the BCF theory.

The edge free energy was not considered in previous works on the kinetic analytical approach, but we can always use the formula (14). In this way we get the same result for the dynamics (22) as in the BCF model, while the result for the dynamics (21) differs very little and the corresponding plots look like those presented in Figs. 4 and 5.
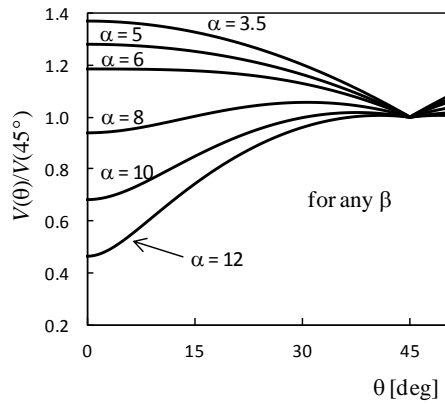
Fig. 6. Normal velocity of a step *V* given by Eq. (28) as a function of the step azimuth θ normalized to the level of velocity for θ = 45°
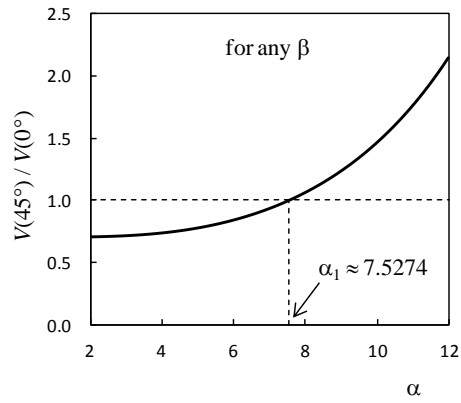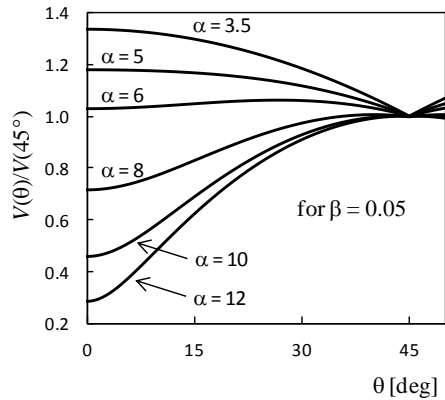

Fig. 7. Ratio of normal velocities *V* given by Eq. (28) for θ = 45° and θ = 0° as a function of the α parameter

Fig. 8. Normal velocity of a step *V* given by Eq. (26) as a function of the step azimuth θ normalized to the level of velocity for θ = 45°

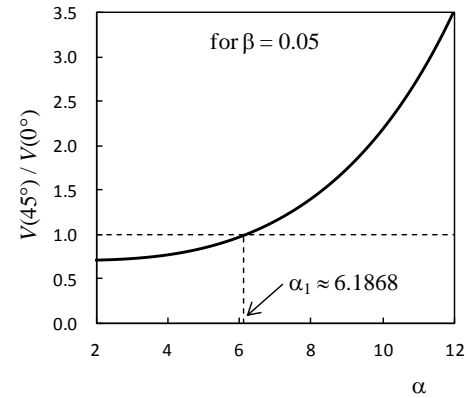Fig. 9. Ratio of normal velocities *V* given by Eq. (26) for θ = 45° and θ = 0° as a function of the α parameter

3.3. Kinetic one-dimensional Monte Carlo simulations

The analytical model presented in section 2.2 has been evaluated in Ref. [5] as consistent for small supersaturations with the results of 1D MC simulations available in Ref. [6]. Because the data available so far were very fragmentary, in this work we present the results of our new simulations.

Comparing the plots in Figs. 10 and 11 with the plots in Figs. 6 and 7, one can notice some discrepancies between the results of 1D MC simulations and the kinetic analytical approach, which are very small for small values of α, but clearly increase with the increase of α. Our MC simulations were performed for $\beta = 0.05$, which may be considered as a small value in terms of crystal growth conditions, but it is also large enough to avoid a strong random dispersion of the results. Since the basic assumptions regarding the geometry of the system and the frequencies of elementary processes (22) are the same in both cases, the discrepancies arise from the assumption (4), which is applied only in the analytical approach.

When the dynamics (21) of elementary events is assumed, the results of 1D MC simulations shown in Figs. 12 and 13 differ only slightly from the predictions of the analytical approach presented in Figs. 8 and 9.
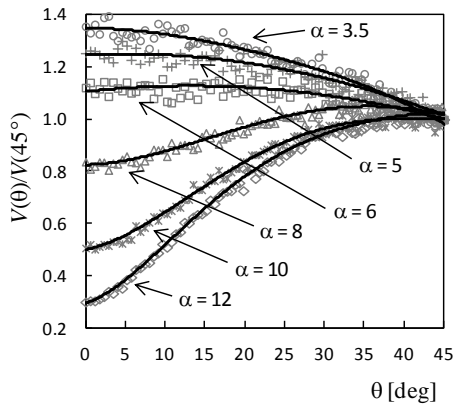

Fig. 10. Normal velocity of a step *V* resulting from Eq. (29) and 1D MC simulations performed for $\beta = 0.05$ and the frequencies (22) as a function of the step azimuth θ. The velocity is normalized to its level for $\theta = 45°$
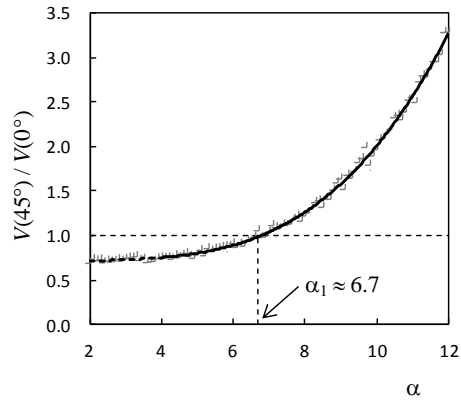
Fig. 11. Ratio of normal velocities *V* resulting from Eq. (29) and 1D MC simulations performed for $\beta = 0.05$ and the frequencies (22) for orientations $\theta = 45°$ and $\theta = 0°$ as a function of the α parameter
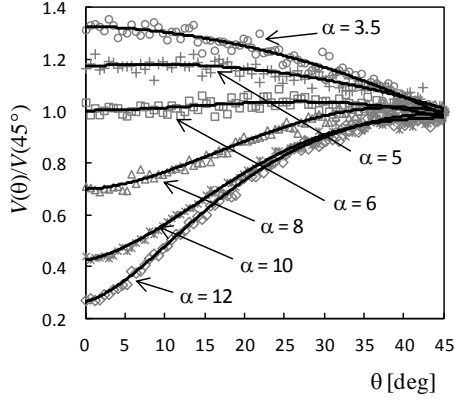
Fig. 12. Normal velocity of a step *V* resulting from Eq. (29) and 1D MC simulations performed for $\beta = 0.05$ and the frequencies (21) as a function of the step azimuth θ. The velocity is normalized to its level for $\theta = 45°$
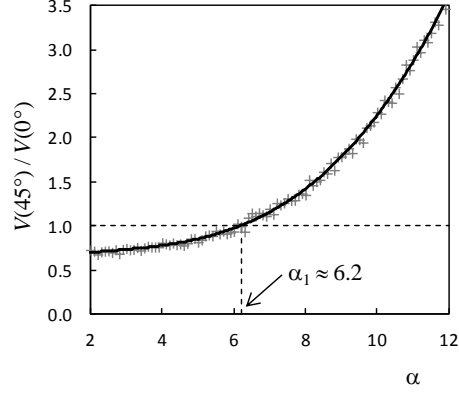
Fig. 13. Ratio of normal velocities *V* resulting from Eq. (29) and 1D MC simulations performed for $\beta = 0.05$ and the frequencies (21) for orientations $\theta = 45°$ and $\theta = 0°$ as a function of the α parameter

4. DISCUSSION

The "solid-on-solid" (SOS) assumption is commonly used in 2D models of the crystal-mother phase interface and does not lead to erroneous predictions in the area of layer-by-layer mechanism of crystal growth. The re-use of the SOS assumption for the second direction leads to a 1D description of the step on the crystal face. This simplification allowed a fully analytical derivation of the normal velocity *V* and of the edge free energy *F* of a straight step moving in any direction θ on the (001) face of Kossel crystal. The $V(\theta)$ and $F(\theta)$ dependencies are necessary, for example, to model the evolution of any step under anisotropic conditions.

However, in the light of the results presented in this paper, all approaches based on one-dimensional description, such as the BCF theory, the kinetic equation and 1D MC simulations, lead to some clearly incorrect predictions:

1) The normal velocity $V(\theta)$ may satisfy relations $V(0°) > V(45°)$, $V(0°) = V(45°)$ or $V(0°) < V(45°)$ depending on the parameters determining crystal growth conditions. The case $V(0°) > V(45°)$, however, is impossible to confirm based on the 2D MC simulations, which show that the spiral growing around a screw dislocation on the (001) face of the Kossel crystal can only be

isotropic or anisotropic with the orientation corresponding to the relation $V(0°) < V(45°)$ depending on the α and β parameters (see, e.g., Refs. [7, 9]).

2) The normal velocity $V(\theta)$ and the edge free energy $F(\theta)$ are not smooth functions for $\theta = 45° + n\,90°$. The functions becomes nearly smooth only for the large values of the Jackson-Temkin parameter $\alpha > 8 \ldots 10$, while the results are clearly unphysical for the remaining values of α in the area of layer-by-layer growth mechanism.

In addition, we must note some other problems appearing in the analytic models that are not directly related to the one-dimensional description of a step:

3) The assumption that there is no correlation between neighbouring kinks may significantly affect the obtained $V(\theta)$ dependency for high values of the α parameter.

4) According to the BCF theory, the entropy of a step was calculated using the Boltzmann formula $S = k_B \ln W$. However, the total energy of all bonds formed by the atoms at the edge of the step may take various levels E_l for the state described by the given set of probabilities $X(k)$. Hence, the probabilities of individual configurations should not be equal, but proportional to $\exp(-E_l/k_B T)$.

The derivation of new analytical dependencies $V(\theta)$ and $F(\theta)$, which should be free of the problems mentioned in points 1-4, is a very complicated task. Hence, it seems that future works should rather focus on determining these dependencies on the basis of 2D MC simulations and finding interpolations for a wide range of crystal growth conditions. This research direction was taken in Refs. [7-9], but the proposed form of the function $V(\theta)$ is inconsistent with the results of MC simulations for large values of θ and the relationship between the parameter of this function and crystal growth conditions is not well defined.

The movement and interaction of spirals on the crystal surface may be studied using 2D MC simulations, however, many interesting results has been also obtained by solving the equation of evolution without considering any microscopic details [10-14]. Unfortunately, recent papers are still based on the isotropic formulation of the problem known from the BCF theory of 1951. In this situation, even the use of rough approximations of the $V(\theta)$ and $F(\theta)$ dependencies could lead to progress in understanding the dynamics of spirals.

Many crystals of key importance for technology can not be described by the Kossel model of crystal. For such crystals Monte Carlo simulations are performed (see, e.g. growth of GaN modelled in Ref. [26]), while the analytical approach is not popular in the literature.

5. CONCLUSIONS

The analysis presented in this paper shows that all one-dimensional models of the step on the crystal surface lead to similar results, which are clearly non-physical for small values of the Jackson-Temkin parameter. The results, however, become more reliable with the increase in the value of this parameter. The obtained dependences can therefore be used with the step evolution equation under strongly anisotropic conditions. This approach seems promising as an extension of many previous works focused only on isotropic conditions.

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WERYFIKACJA JEDNOWYMIAROWYCH MODELI OPISUJĄCYCH ANIZOTROPIĘ STOPNIA WZROSTU

Streszczenie

Dokonano przeglądu modeli znanych z literatury, które umożliwiają otrzymanie kierunkowych zależności prędkości normalnej prostoliniowego stopnia wzrostu na ścianie (001) kryształu Kossela oraz jego krawędziowej energii swobodnej. Zależności zostały rozważone w szerokim zakresie warunków wzrostu kryształu, co umożliwiło ukazanie niezgodności pomiędzy modelami oraz ograniczeń w zakresie ich stosowalności. Przedstawione wyniki koncentrują się na jednowymiarowych kinetycznych i termodynamicznych modelach pojedynczego stopnia wzrostu.