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# Model for growth of fractal solid state surface and possibility of its verification by means of atomic force microscopy

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**Abstract.** In the paper, methods of verification of models for growth of solid state surface by means of atomic force microscopy are suggested. Simulation of growth of fractals with cylindrical generatrix on the solid state surface is presented. Our mathematical model of this process is based on generalization of the Kardar-Parisi-Zhang equation. Corner stones of this generalization are both conjecture of anisotropy of growth of the surface and approximation of small angles. The method of characteristics has been applied to solve the Kardar-Parisi-Zhang equation. Its solution should be considered up to the gradient catastrophe. The difficulty of nondifferentiability of fractal initial generatrix has been overcome by transition from a mathematical fractal to a physical one.

## 1. Introduction

Since the last quarter of the twentieth century, scanning probe microscopy (SPM) has broadened extensively because of arising of new research methods, such as piezoresponse force microscopy, apertureless scanning near-field optical microscopy, magnetic resonance force microscopy, and so on. Nowadays, the area of applications of SPM includes solid state physics, biology, mineralogy, etc. But since the progress in functional analysis, image processing, and computer technique is considerable, atomic force microscopy (AFM) invented by G. Binnig, C.F. Quate, and C. Gerber in 1986 did not exhaust its possibilities yet, because using of AFM allows us to select adequate models for growing surface of the solid state.

Let us demonstrate this idea on the example of the Kardar-Parisi-Zhang equation (KPZ) [1]:

$$\frac{\partial z}{\partial t} = c \cdot \sqrt{1 + (\nabla z)^2} + \mu \cdot \nabla^2 z + Q(x, y, t). \quad (1)$$

The KPZ-equation has been applied to modelling of the process of sputtering of a substance on a surface of solid state [1]. In equation (1),  $z$  is the height of the surface – in general case, it is a function of coordinates  $z(x, y, t)$ ;  $\nabla$  is two-dimensional gradient. The first term on the right-hand side of equation (1) shows that the growth of the surface occurs at a constant surface growing rate  $c$  strictly along the local normal to it. The second term on the right-hand side describes relaxation of the surface by a surface tension  $\mu$ . At last,  $Q(x, y, t)$  is an extra source of particles deposition.



Equation (1) should be provided by initial condition:

$$z(x, y, 0) = z_0(x, y), \quad (x, y) \in D \subset R^2, \quad (2)$$

corresponding to initial shape of the surface under investigation.

It is clear that function (2) in domain  $D$  can be measured by means of AFM. After the finish of the sputtering process at the moment of time  $t = T$  the height  $\tilde{z}(x, y, T)$  of the surface in domain  $D$  can be estimated by AFM again. On the other hand, starting from initial condition (2), one can solve the KPZ-equation (1) numerically on the interval of time  $t \in [0, T]$  and derive the theoretical height  $z(x, y, T)$  of the surface at  $t = T$ . Therefore, we can compare these two heights in some norm, for instance in the functional space  $C(\bar{D})$  of functions continuous on  $\bar{D}$ :

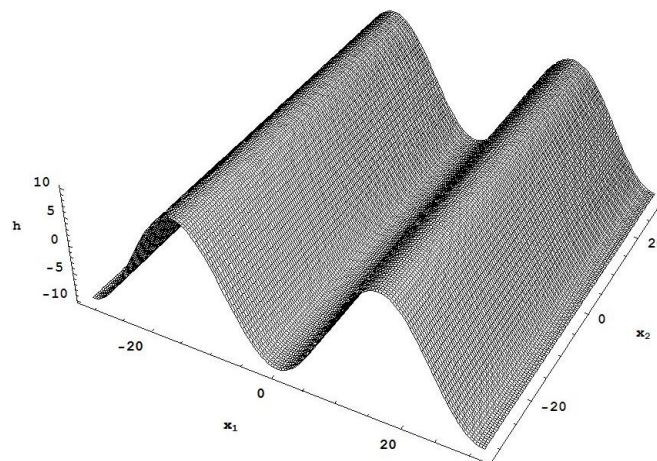
$$\|z - \tilde{z}\| = \sup_{(x, y) \in D} |z(x, y, T) - \tilde{z}(x, y, T)|. \quad (3)$$

If number (3) is greater than some earlier chosen threshold value, then one claims that the theoretical model of growth is wrong; hence, it should be rejected or modified. Thus, in order to use this method of comparison of the theory and experiment, it is required to develop various generalizations of the KPZ-equation (1).

For simplicity in this paper, we confine ourselves to an analysis of the growth of a surface with a cylindrical generatrix (Fig. 1).

It is necessary to note here that fractal phenomena are sure to be widespread in physics of solid state. In particular, in work [2] based on the study of the surface images obtained with AFM for a number of samples of structural materials subjected to typical physical-chemical processing, such as microarc oxidation, diamond grinding etc., it is uniquely shown that the investigated surfaces are fractal. Effects of fractality on surface of nanostructured semiconductors have been described in [3]. Formation of fractal patterns on the surface of nanocomposite materials is under investigation in [4]. In [5], it is proved that in metals the surface layer has a fractal structure. It is obvious that there are some features under solution of the KPZ-equation (1) with fractal initial condition (2) in comparison with the same one with smooth initial condition (2).

The rest of the article is organized as follows: in Section 2 we demonstrate how to construct the generalized KPZ-equation in approximation of small angles taking into account the assumption about the anisotropy of the surface growth [6]. Section 3 deals with the regularized Darboux function. Peculiarities of mathematical modeling of the growth of the fractal surface in the framework of the method of characteristics are under consideration in Section 4. Perspectives of further investigations are also discussed.



**Figure 1.** A surface with a cylindrical generatrix.

## 2. Derivation of generalized KPZ-equation in the framework of approximation of small angles

The aim of this section is to obtain a nonlinear partial differential equation of the first order for the height of anisotropically growing surface. In this case, the generalized KPZ-equation has the form [7]:

$$\frac{\partial z}{\partial t} = V(\theta) \cdot \left[ 1 + \left( \frac{\partial z}{\partial x} \right)^2 \right]^{\frac{1}{2}}, \quad z(x,0) = z_0(x), \quad x \in R, \quad (4)$$

where  $z(x,t)$  – the height of growing surface with a cylindrical generatrix,  $V(\theta)$  – the rate of its growth, which depends on the angle  $\theta$  between the local normal to the surface and the z-axis, and  $z_0(x)$  is initial shape of the surface under investigation. Surface tension and extra source are not considered in this model.

Wherein

$$V(\theta) = \int_{\theta_-(\theta)}^{\theta_+(\theta)} D(\theta') \cdot \cos(\theta - \theta') \cdot d\theta', \quad (5)$$

where  $D(\theta)$  – a directivity diagram that determines the intensity of the flow of particles falling out on the growing surface [7], functions  $\theta_{\pm}(\theta)$  take into account the shading effects of the rest of the profile  $z(x,t)$ , and angle  $\theta$  is related to the profile under consideration by the next relation [7]:

$$\tan \theta = -\frac{\partial z}{\partial x}. \quad (6)$$

The anisotropy of the growth of the surface is considered by means of the following expression for the directivity diagram:

$$D(\theta) = D_0 + D_2 \cdot \cos^2 \theta, \quad D_0 > 0, \quad D_2 > 0. \quad (7)$$

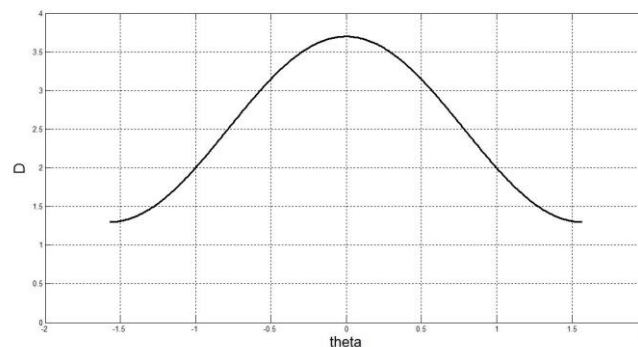
A typical graph of such directivity diagram is presented in Figure 2.

At first, let us calculate the rate (5) of surface growth in our case. Suppose that there is no shading by further parts of generatrix  $z(x,t)$ , then the limits of integration in formula (5) are equal to:

$$\theta_-(\theta) = \begin{cases} \theta - \pi/2, & \theta > 0 \\ -\pi/2, & \theta < 0 \end{cases} \quad \theta_+(\theta) = \begin{cases} \pi/2, & \theta > 0 \\ \pi/2 + \theta, & \theta < 0 \end{cases}. \quad (8)$$

Combining expressions (5), (7), and (8) we find that:

$$V(\theta) = D_0 \cdot (1 + \cos \theta) + \frac{D_2}{3} \cdot (1 + \cos \theta)^2. \quad (9)$$



**Figure 2.** Angular dependence of directivity diagram.

Secondly, applying connection (6) between angle  $\theta$  and generatrix  $z(x,t)$  one can rewrite equation (4) as follows:

$$\frac{\partial z}{\partial t} = D_0 + \frac{2 \cdot D_2}{3} + \left( D_0 + \frac{D_2}{3} \right) \cdot \left[ 1 + \left( \frac{\partial z}{\partial x} \right)^2 \right]^{\frac{1}{2}} + \frac{D_2}{3} \cdot \left[ 1 + \left( \frac{\partial z}{\partial x} \right)^2 \right]^{-\frac{1}{2}}. \quad (10)$$

After that let us assume that  $|\theta| \ll 1$ . This is the so-called approximation of small angles. In the framework of this approximation  $|\partial z / \partial x| \ll 1$ . Hence, using Taylor expansion of the right side of equation (10) and rejecting terms with powers of  $\partial z / \partial x$  greater than four we can simplify this equation in the next manner:

$$\frac{\partial z}{\partial t} = 2 \cdot D_0 + \frac{4 \cdot D_2}{3} + \frac{D_0}{2} \cdot \left( \frac{\partial z}{\partial x} \right)^2 + \frac{2 \cdot D_2 - 3 \cdot D_0}{24} \cdot \left( \frac{\partial z}{\partial x} \right)^4. \quad (11)$$

One can eliminate homogeneous growth of the surface from equation (11) by trivial substitution:

$$z(x,t) = \left( 2 \cdot D_0 + \frac{4 \cdot D_2}{3} \right) \cdot t + h(x,t), \quad (12)$$

which leads to the following Cauchy problem for new unknown function  $h(x,t)$ :

$$\frac{\partial h}{\partial t} = \frac{D_0}{2} \cdot \left( \frac{\partial h}{\partial x} \right)^2 + \frac{2 \cdot D_2 - 3 \cdot D_0}{24} \cdot \left( \frac{\partial h}{\partial x} \right)^4, \quad h(x,0) = z_0(x). \quad (13)$$

We underline that in order to get contributions of the same order from both the first and the second terms in the right side of equation (13) the inequality  $D_2 \gg D_0$  ought to be true.

Let us choose for initial condition for equation (13) typical values of its amplitude  $A$  and spatial scale  $L$  namely:

$$z_0(x) = A \cdot h_0(x/L), \quad (14)$$

where  $h_0(\dots)$  is dimensionless function then rescaling time  $t$ , coordinate  $x$ , and nonhomogeneous height of growing surface  $h$  as  $\frac{A \cdot D_0 \cdot t}{L^2} \rightarrow t$ ,  $\frac{x}{L} \rightarrow x$  and  $\frac{h}{A} \rightarrow h$  we reduce equation (13) and its initial condition (14) to the dimensionless form:

$$\frac{\partial h}{\partial t} = \frac{1}{2} \cdot \left( \frac{\partial h}{\partial x} \right)^2 + \frac{g}{4} \cdot \left( \frac{\partial h}{\partial x} \right)^4, \quad h(x,0) = h_0(x), \quad (15)$$

where  $g = \frac{2 \cdot D_2 - 3 \cdot D_0}{6 \cdot D_0} \cdot \frac{A^2}{L^2}$  is a positive coupling constant.

The solution of Cauchy problem (15) by the method of characteristics (see [7] and references therein) is equal to:

$$x = y + (1 + g \cdot u_0^2(y)) \cdot u_0(y) \cdot t \quad h = h_0(y) - \left( \frac{1}{2} + \frac{3}{2} \cdot g \cdot u_0^2(y) \right) \cdot u_0^2(y) \cdot t, \quad (16)$$

where  $u_0(y) = -h'_0(y)$ .

### 3. The regularized Darboux function as an example of physical fractal

It is well-known that fractal functions are continuous nowhere differentiable ones (see [8] and references therein). The formulas (16) for solution of nonlinear partial differential equation (15) include not only the initial profile  $h_0(x)$ , but also its derivative  $h'_0(x)$ . This means that to describe

the growth of fractal surfaces within the framework of the approach developed in the previous Section, the fractal initial profile must undergo some regularization.

The conceptual basis of this regularization is known to include in transfer from mathematical fractals to physical fractals [8]. The scheme of this transfer is presented in Figure 3. We stress that this scheme was approved by B. Mandelbrot [9].

In order to illustrate this approach by concrete example, let us consider the Darboux function [8]:

$$D(x) = \sum_{n=1}^{\infty} \frac{\sin[(n+1)!x]}{n!}. \tag{17}$$

This function is nondifferentiable for all real numbers [8]; however, if we take only a limited number  $N$  of terms of the series (17), then the resulting function:

$$D_N(x) = \sum_{n=1}^N \frac{\sin[(n+1)!x]}{n!} \tag{18}$$

will be differentiable as many times as required.

Error  $\varepsilon_N$  of this approximation:

$$|D(x) - D_N(x)| \leq \varepsilon_N, \tag{19}$$

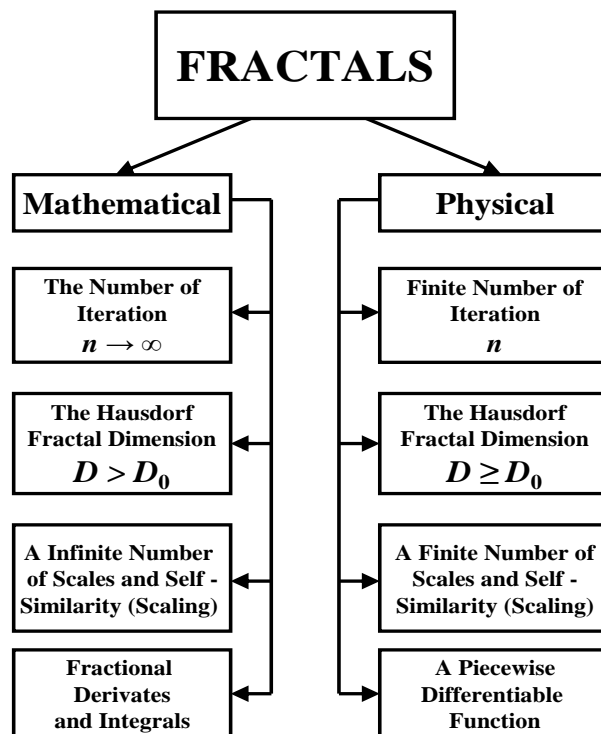
can be easily estimated with help of inequality  $|\sin x| \leq 1$  which is valid for all real  $x$  namely

$$\varepsilon_N = \sum_{n=N+1}^{\infty} \frac{1}{n!} \tag{20}$$

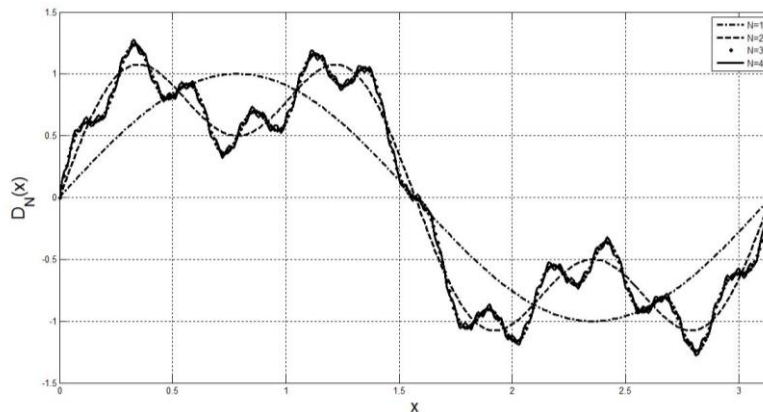
For sum (20) from any course of calculus the following inequality is well known:

$$\varepsilon_N \leq \frac{1}{N!N} \tag{21}$$

Thus, from the formula (21) one can see that under quite large  $N$  error of approximation of the Darboux function (17) by means of truncated functional series (18) becomes quite small.



**Figure 3.** The Potapov scheme of mathematical and physical fractals.



**Figure 4.** The regularized Darboux functions for  $N = 1, 2, 3, 4$ .

Graphs of the regularized Darboux functions (18) for  $N = 1, 2, 3, 4$  are shown in Figure 4. One can observe that there are no sharp distinctions between  $D_3(x)$  and  $D_4(x)$  yet.

The regularized Darboux function possesses by the following derivative:

$$D'_N(x) = \sum_{n=1}^N (n+1) \cdot \cos[(n+1)!x]. \quad (22)$$

It is obvious that there is the next inequality for upper bound of function (22):

$$|D'_N(x)| \leq \frac{N \cdot (N+3)}{2}, \quad (23)$$

Therefore, absolute value of the derivative of the regularized Darboux function grows as  $O(N^2)$  when  $N$  tends to infinity. This circumstance seems to look like violation of correctness of approximation of small angles, but we emphasize that there is no contradiction indeed, because requirement  $|\partial h / \partial x| \ll 1$  was imposed on dimensionfull variables in dimensionfull equation (13). It means that in accordance with inequality (23) for self-consistency of our assumptions typical values of amplitude  $A$  and spatial scale  $L$  of dimensionfull initial condition (14) ought to obey to the following inequality:

$$\frac{A \cdot N \cdot (N+3)}{2 \cdot L} \ll 1. \quad (24)$$

#### 4. Results of numerical simulation

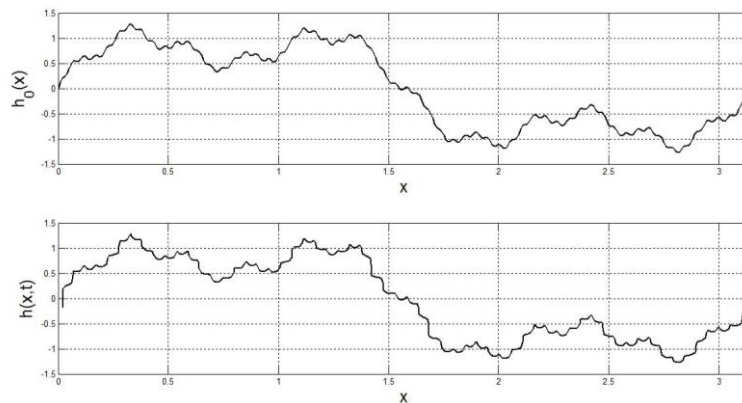
Let us now demonstrate the results of numerical modeling for the above developed approaches.

As a dimensionless initial condition, the regularized Darboux function (18) under  $N=4$  was chosen:

$$h_0(x) = D_4(x). \quad (25)$$

In this case, the error of approximation of mathematical fractal (17) by physical fractal (25) is equal or less than  $1/96$ :  $\varepsilon_4 \leq 1/96 \approx 0.0104$ . This level of error is expected to be appropriate for rigor of our consideration. Further, due to periodicity of initial condition (25) namely  $D_4(x + \pi) = D_4(x)$  we can restrict ourselves by the investigation of the behavior of the surface over the segment  $[0, \pi]$  of the  $x$ -axis without loss of generality. Value of coupling constant is equal to  $g=0.01$ .

The initial condition (25) and the result of its temporal evolution at  $t=0.0005$  are presented in Figure 5 above and below, respectively. From this Figure, one can see that temporal evolution leads to narrowing of the profile of the surface in the neighborhood of local maxima of the function  $h(x, t)$ .

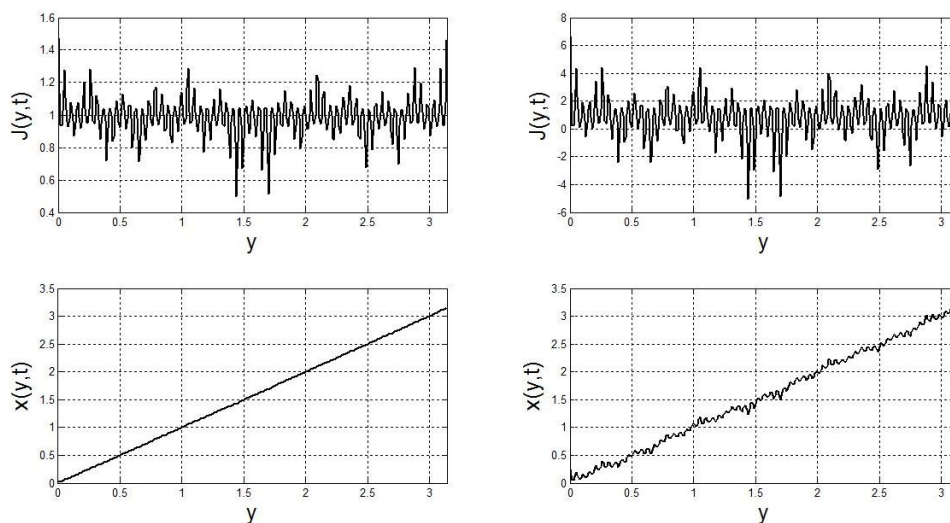


**Figure 5.** Initial height of cylindrical generatrix (above) and result of its temporal evolution until gradient catastrophe (below).

We underline that researchers ought to be neat and careful under operating with equation (15), because representation (16) of solution of this equation is applicable only up to the moment of gradient catastrophe. At this moment of time, one-to-one correspondence  $y(x,t)$  between Eulerian coordinate  $x$  and Lagrangian coordinate  $y$  in accordance with the first formula in formula (16) is violated. In order to determine moment of gradient catastrophe for fixed initial profile, it is necessary to watch zeroes of the following Jacobian:

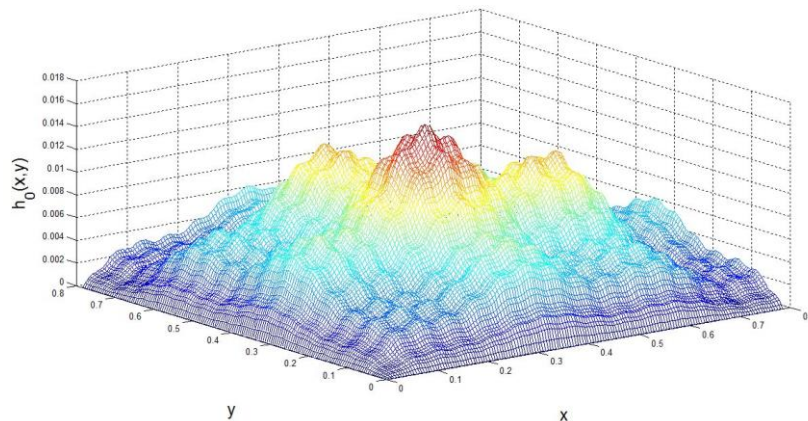
$$J(y,t) \equiv \frac{\partial x(y,t)}{\partial y} = 1 + (1 + 3 \cdot g \cdot u_0^2(y)) \cdot u_0'(y) \cdot t. \tag{26}$$

This untrivial situation is illustrated by Figure 6. On the left side of Figure 6  $J(y,t)$  and  $x(y,t)$  at  $t=0.0005$  corresponding to Figure 5 are presented. In this case, Jacobian (26) is positive everywhere  $J(y,t) > 0$  and, therefore, function  $y(x,t)$  is one-to-one mapping. On the right side of Figure 6,  $J(y,t)$  and  $x(y,t)$  at  $t = 0.006$  are presented. In this case, one can observe that there are a lot of zeroes of Jacobian (26) and, hence,  $y(x,t)$  is multifunction, evidently. It means that at  $t = 0.006$  instead of equations (16) one ought to deal with the so-called weak solutions of equation (15) constructed in the framework of the Oleynik-Lax absolute minimum principle or the E-Rykov-Sinai global principle (see [7] and references therein).



**Figure 6.** Dependences of Jacobian and Eulerian coordinate on Lagrangian coordinate before (on the left side) and after (on the right side) of gradient catastrophe.





**Figure 7.** The two-dimensional regularized Darboux function.

The aim of further investigation is thought to extend the approach elaborated above on general two-dimensional situation both before and after gradient catastrophe. For instance, in two-dimensional case the initial profile (18) can be generalized as follows:

$$h_0(x, y) = D_N(x) \cdot D_N(y). \quad (27)$$

Physical fractal (27) under  $N=5$  is shown in Figure 7.

After that, fractal dimension of growing surface ought to be calculated in accordance with solution of the two-dimensional generalized KPZ-equation by methods developed earlier [8]. One can compare the obtained result with estimation of fractal dimension based on data of AFM for the surface under investigation. Another way of comparison of the theory and AFM-measurements is to investigate connections between fractal properties of the surface of solid state and scattering data on this surface of electromagnetic and elastic waves [10]. Beyond any doubt both of these criteria ought to be analyzed simultaneously with norm (3). In order to broaden sphere of applications of the suggested verification procedure, we also intend to consider other examples of equations describing the growth of surface of solid state, for instance the Bradley-Harper equation [11], which is a nonlinear mathematical model for the formation of an inhomogeneous topography on the surface of solid state under ionic bombardment.

## 5. Conclusion

In the article, procedure of verifying models of growth of solid state surface and selecting the true ones with support of this process by AFM has been considered. To realize the procedure in practice, the exact solution of the generalized KPZ-equation describing anisotropic growth of the surface with cylindrical generatrix until the gradient catastrophe has been constructed in the framework of approximation of small angles. In order to demonstrate efficiency of the suggested procedure, the regularized Darboux function has been chosen as the initial generatrix.

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