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PHASE FIELD MODELING OF MOVING SURFACE ROUGHNESS PROFILE

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Abstract: In this paper we propose a new model of crystallization, in view of deposition of particles on the surface, based on the theory of phase field is considered to be characteristic of this model depending on parameters. Numerically solve the problem of heat transfer with moving boundary. Estimates are given for for the fractal dimension of the sample surface, described by the proposed model. The proposed model can be applied to solve various technical problems.

Key Words: phase-field model, the problem with moving boundary, rough surface

1. Introduction

The actual physical bodies have complex surfaces, which is especially important in connection with the development of technology that uses nano-objects. Surface roughness is defined as a set of surface roughness with relatively small increments in the base length.

The type and properties of the surface roughness of machine parts significantly determine their performance characteristics, durability, strength. The shape of the roughness elements, their distribution in the treated area are very different from the traditional view of them as the alternation of ridges and valleys that will take into account in the investigation of structural materials. Significantly influence the design of the roughness of the contact interaction

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[1]. Roughness also be taken into account in problems associated with magnetic nanostructures, as well as the effect of roughness on the deposition rate of aerosol on the surface.

There are many approaches to modeling the surface, ranging from discrete models to the statistical (probability theory) or fractal [2]. One of the most important properties of a surface is its self-similar nature, which gives reason for her modeling in the form of a fractal object. This approach has wide application in various fields [1,3,4].

Modeling of surfaces with fractal properties relevant to the problems with moving boundaries. Appearance of the surface over time is determined by the mechanisms of growth, and retains its properties at each step of the process. For example, if the aerosol deposition on the surface or deposition of particles, there are complex structures on the surface, which can be modeled as a fractal object [5].

There is a class of models, where the surface is represented as a functional [2]. One of the parameters of this model is the fractal dimension, this approach is well applicable in problems with fixed boundaries, the problems of friction, the contact interaction. The parameters of these models the surface of the material can be determined on the basis of the data measurement profilograms surface of the material [6-7].

Processes with moving boundaries, such as deposition of nanoparticles on the surface can be described by fractal models of growth, where surface appearance is constantly changing. In these models the surface (or surface profile) is usually determined by the solution of stochastic differential equations [8-9]. The main mechanism of growth in such models is the random deposition of particles, while the models do not take into account the thermodynamic characteristics of the system.

In many real physical processes, such as formation of ice crystals (snowflakes, icicles, etc.), the shape of the surface varies not only by the deposition of particles of small size but also due to the processes of phase transformation [10-12]. The phase boundary can be represented in the idea of a fractal object (snowflake, etc.). Modeling of processes of change of phase boundaries leads to the Stefan problem. In this task under a wide class of Stephen understood mathematical models describing the heat, and diffusion processes accompanied by phase transformations and the environment by absorption or release of latent heat. These processes occur in metallurgy, crystal growth, as well as in several other areas of science. The most characteristic feature of these processes, because of their mathematical models are not linear and difficult to analyze, are unknown in advance ("free") the boundaries between different phases.

One of the alternative models of the crystallization process, which appeared and rapidly developing in recent years, a phase-field model [13]. As shown in several studies, the phase-field model under certain limiting values close to the classical formulation of the Stefan problem (with a clearly defined boundary) [14].

The paper contains a modified model of the crystallization process, taking into account particle deposition on the surface, based on the theory of phase field. Such a model can be used to represent the actual surface of the body for a wide class of problems. Unlike other models of this kind is that it takes into account the effect of deposited particles at the phase boundary explicitly.

2. Basic Model

Consider the class of models describing the crystallization of a moving interphase boundaries [10-11]. There are several models of phase field describing phenomena such as crystallization, solidification of a pure material from its undercooled melt. These models are based on the introduction of the spatial variable phase field $p(x, y, t)$ as a function of horizontal and vertical coordinates x and y with time t, which characterizes the state of matter, and taking different values for the solid and liquid phases (1 and 0). We denote the main steps to obtain the equations describing the system. We write the free energy of a thermodynamic potential in the Landau-Ginzburg

$$\Phi(p, m) = \int F(p, m) + \frac{\varepsilon^2(\nabla p)^2}{2} dV$$

For two-phase system, the function $F(p, m)$ at constant temperature is a model potential with two local minima at p, it is sometimes called the synergistic potential. If the write function of the form

$$F(p, m) = \frac{1}{4}p^4 - (\frac{1}{2} - \frac{1}{3}m)p^3 + (\frac{1}{4} - \frac{1}{2}m)p^2$$

Given $\tau\frac{\partial p}{\partial t} = -\frac{\delta\Phi}{\delta p}$ obtained

$$\tau\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}(\varepsilon\varepsilon'\frac{\partial p}{\partial y}) + \frac{\partial}{\partial y}(\varepsilon\varepsilon'\frac{\partial p}{\partial x}) + \nabla(\varepsilon^2\nabla p) + p(1-p)(p - \frac{1}{2} + m) \quad (1)$$

In [10] proposed the functional relations for the values of variables in the equation for describing the growth dendride structures. These dependencies describe the anisotropy of the material and the effect of temperature on growth

$$\varepsilon(\theta) = \varepsilon(1 + \delta cos[j(\theta - \theta_0)]),$$

$$m(T) = \frac{\alpha}{\pi} arctg[\gamma(T_e - T)].$$

Here ε - by appropriate parameter value of the transition layer, values δ and j characterize the average intensity and anisotropy of the main number, θ - the angle between the gradient of the p and chosen one of the axes of the coordinate system, T_e - meaning the value of the equilibrium temperature (reduced to dimensionless form), α, γ - are positive constants ($\alpha < 1$) [10,15]. For the dimensionless temperature equation can be written

$$\frac{\partial T}{\partial t} = \nabla^2 T + K \frac{\partial p}{\partial t} \tag{2}$$

The resulting system of two equations - a system for temperature and the phase variable. Such systems type describe the growth of dendritic structures.

3. New Model

In this paper we propose to consider the parameter K as a function of time and coordinates $K(x,t)$. This function must have the properties of continuity and boundedness. Representation in the form of the function has the following physical meaning. In the case of sedimentation of particles of different sizes on the surface, a fixed interval of the surface is changed to a discrete value for a small period of time, due to the fact that the deposited particles have a finite size. Similarly, the formation of clusters on the surface.

Consider a simple example, then generalize the function $K(x,t)$. Let l,h,ε - parameters characterizes the form of function, k_1 and k_2 - maximum and minimum values. Denote the following sets:

$$K_1(x,t) = \{(x,t)| - l/2 < x < l/2, 0 < t < h(1 - 2|x|/l)\} \tag{3}$$

$$K_2(x,t) = \{(x,t)| - l(1 + \varepsilon/h)/2 < x < l(1 + \varepsilon/h)/2, \\ -\varepsilon < t < h(1 - 2|x|/l) + \varepsilon\sqrt{1 + (2h/l)^2}\} \tag{4}$$

$$K_3(x,t) = \{(x,t)|(x,t) \in (K_2/K_1), x > 0, \\ t > -2h(x - \varepsilon)/(l(1 + \sqrt{1 + (2h/l)^2}))\} \tag{5}$$

$$K_4(x,t) = \{(x,t)|(x,t) \in (K_2/K_1),$$
$$t < Min(-2h(x-\varepsilon)/(l(1+\sqrt{1+(2h/l)^2}),$$
$$0, 2h(x+\varepsilon)/(l(1+\sqrt{1+(2h/l)^2}))\} \quad (6)$$
$$K_5(x,t) = \{(x,t)|(x,t) \in (K_2/K_1),$$
$$t > 2h(x+\varepsilon)/(l(1+\sqrt{1+(2h/l)^2})\} \quad (7)$$

Let $K(x,t)$ be defined as follows

$$S(x,t) = \begin{cases} k_1 & , \text{for } (x,t) \in K_1 \\ (\frac{2h}{l}x + t - h)\frac{k_2-k_1}{\varepsilon(1+\sqrt{1+(2h/l)^2})} & , \text{for } (x,t) \in K_3 \\ -\frac{t(k_2-k_1)}{\varepsilon} + k_1 & , \text{for } (x,t) \in K_4 \\ (-\frac{2h}{l}x + t - h)\frac{k_2-k_1}{\varepsilon(1+\sqrt{1+(2h/l)^2})} & , \text{for } (x,t) \in K_5 \\ k_2 & , \text{for } (x,t) \notin K_2 \end{cases} \quad (8)$$

$$g(x) = k_1 + (k_2 - k_1)(1 - cos(\pi(x-k_1)/(k_2-k_1)))/2$$
$$K(x,t) = g(S(x,t)) \quad (9)$$

Thus, we define a disturbance of the function $K(x,t)$ on the set of (x,t) with the center in the neighborhood of $(0,0)$. Solution to the problem of two equations in this neighborhood vary slightly. Further, define a series of disturbances at different points in area (x,t), it will make a greater contribution in the form of the solution. Consider the region $\Omega = \{(x,t)|0 < x < K, 0 < t < t_f\}$, we select a subset of rectangles in $R_i = \{(x,t)|x_{0i} < x < x_{0i} + a_i, y_{0i} < y < y_{0i} + b_i\}$, so that (1)$\forall i : R_i \subset \Omega$, (2) $\forall i_1, i_2 : R_{i_1} \cap R_{i_2} = \emptyset$. Bases such rectangles is a random variable $a_i = \xi_1$ and altitude $b_i = C_1 a_i + C_2$.

Here are a few possibilities of filling:

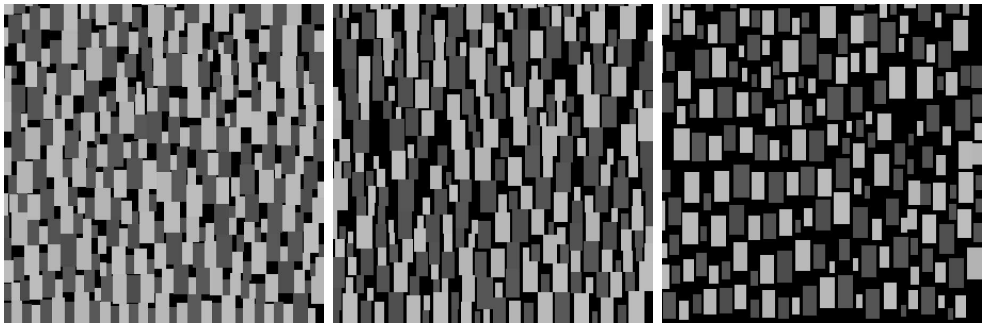
(a) Any rectangle should have common points at each of its other side. Filling area will be below, at the same time $x_{0i+1} = x_{0i} + a_i$, $x_{0i=0} = 0$, If at some step $x_{0i} + a_i > K$ resets $x_{0i} = 0$. Example, Figure 1(a).

(b) Filling area will be below, at the same time $x_{0i+1} = x_{0i} + \xi_2$, $x_{0i=0} = 0$, If at some step $x_{0i} + a_i > K$ resets $x_{0i} = 0$. Example, Figure 1(b).

(c) Filling area will be below, at the same time $x_{0i+1} = x_{0i} + \xi_2$, $x_{0i=0} = 0$, If at some step $x_{0i} + a_i > K$ resets $x_{0i} = 0$. When filling in a single layer, to the maximum possible value of height adds another ξ_3. Example, Figure 1(c).

The first two points are special cases of the third, for the values of the function equal to 0. Obtain the shape and form of distribution, and hence the further construction of $K(x,t)$, determined by the distributions ξ_1, ξ_2, ξ_3.

Next, we assume the distribution functions ξ_1, ξ_3 are uniform, denoted, $\xi_1 \sim U(min_1, max_1)$, $\xi_3 \sim U(min_3, max_3)$, ξ_2 value is the log-normal or gamma distribution, denoted by $\xi_2 \sim LogN(\mu, \sigma^2)$, $\xi_2 \sim \Gamma(k, \theta)$. The distribution law of value ξ_2, due to the fact that the particle size distribution for many types of aerosols has this form [16].



a) b) c)

Figure 1: (a-c) in the plane (x, t) are shown in gray rectangular subset described above, in all three cases the value ξ_1, ξ_2, ξ_3 have a uniform distribution.

We define a function $K(x,t)$ on Ω, we denote $K_\Omega(x,t)$. To begin to define $K(x,t)$ on R_i, for all i, denoted by $K_{R_i}(x,t)$.

$$K_{R_i}(x,t) = \begin{cases} k_1 & \text{, for } t < h(a_i)(1 - 2|x - (x_{0i} + a_i/2)|/a_i) \\ +b_i & \\ k_2 & \text{, for } t \geq h(a_i)(1 - 2|x - (x_{0i} + a_i/2)|/a_i) \\ +b_i & \end{cases} \tag{10}$$

$$K_\Omega(x,t) = \begin{cases} K_{R_i}(x,t) & \text{, for } (x,t) \in R_i \\ k_2 & \text{, otherwise} \end{cases} \tag{11}$$

We assume that $h(x)$ has the following form $h(x) = xtg(p_1 \sin^s(x/2) + p_2)$.

ε	α	γ	T_e	k_1	k_2	C_1	C_2	p_1	s	p_2
0.01	4.0	10	1	2.0	0.8	17	50	0.23	0.65	0.01

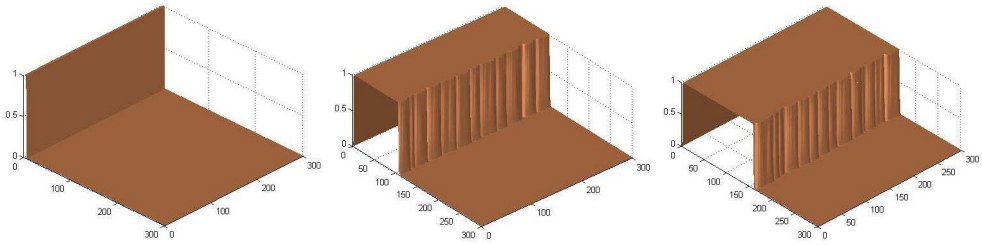
Table 1: values of the constants.

We consider in $\Omega_{xy} = \{(x, y, t)|0 < x < K, 0 < y < L, 0 < t < t_f\}$ problem of the following types:

$$\tau \frac{\partial p}{\partial t} = \nabla(\varepsilon^2 \nabla p) + p(1-p)(p - \frac{1}{2} + m)$$

$$\frac{\partial T}{\partial t} = \nabla^2 T + K_\Omega \frac{\partial p}{\partial t}$$

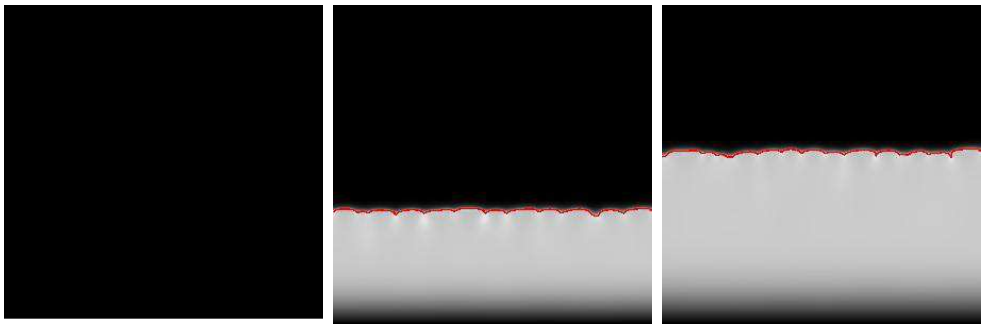
With the initial conditions, the phase variable $p(x, 0, 0) = 1$,$p(x, y, 0) = 0$, and the dimensionless temperature $T(x, 0, 0) = 1$,$T(x, y, 0) = 0$. For the numerical solution of the problem, we use the explicit scheme with steps on the grid $\triangle x = \triangle y = 0.01$, time step $\triangle t = 0.0002$. The parameters of the distribution functions can be selected depending on the context of the problem, from this solution has different properties. The values used for constants of the equations are given in the Table 1. Figure 2-3 shows the values of the phase variable and the dimensionless temperature, which describe the profile at regular intervals. The sample values are equal $min_1 = min_3 = 0$, $max_1 = max_3 = 20$, the value of the parameters of the log-normal distribution (μ, σ), respectively $(2.4, 0.7)$.



a) b) c)

Figure 2: graphs show the value of the phase variable in the solution at the initial time (a), and at regular intervals (b), (c).

In this paper we consider the surface of the samples of "chrome on glass," and "gold on silicon." The data were obtained by scanning tunneling microscopy. Sample sizes: chromium on glass - 2*2mcm, gold on silicon - 5*5mcm. The data were provided Nanolaboratoriey "Inzhekon" Tver. Features tunneling microscope field scanning (dimensions of the test sample) - 5 * 5mcm; Scanning step in the sample (minimum displacement of the probe in the sample plane) - 0.08nm, measuring step Vertical - 0.02nm altitude range - 10,2mcm. To study the fractal properties of the surfaces of the samples, as well as that would assess the nature of the relief surfaces were calculated values of Hurst exponent. From



a) b) c)

Figure 3: figures are shown in white value of the dimensionless temperature in the solution at the initial time (s), and at regular intervals (b), (c). Red marked boundary between the phases ($0.05 < p < 0.95$).

the value of index H (Hurst coefficient) can be concluded about the nature of the data in the study sample. Thus, by introducing the sequence of applying the method of least squares, we find the slope of the line passing as close to the obtained points. In [6,7] based on R/S-analysis of the samples were profilograms surfaces, a description of the surface microrelief, as well as outline the rationale for the relationship between processing parameters and values of the fractal dimension of the surface. Based on the calculation of R/S statistics for a set series of height values profiles obtained with a scanning microscope, values have been estimated Hurst exponent for the profiles of the surfaces of the samples. The average value of Hurst exponent for the level curves of solutions, for these parameters, in agreement with experimental results.

4. Conclusion

In this paper we proposed a new model of phase field, which can be used for modeling with a moving boundary, such as crystallization, and to describe the surface of real bodies.

Performed numerical experiment on the calculation of the temperature field near a rough surface. A new mathematical model of the crystallization process, taking into account the deposition of particles on the surface, based on the theory of phase field. Conducted experiments to study the geometry of the surface of nanomaterials using a scanning tunneling microscope, a distinctive feature of which is to obtain data of surface roughness. The results of numerical

simulation showed that the value of Hurst exponent for real samples with the values obtained in the simulation.

The proposed model can be applied in solving problems related to the creation of new materials with desired properties, in problems of contact interaction of machine parts, as well as in the problems of estimating the rate of deposition of aerosol particles on the surface.

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