

On some Mathematical Models of Growth of Solid Crystals and Nanowires

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In this paper some aspects related to the crystal growth are considered. This process is described by non-linear reaction-diffusion equation with the specific initial-boundary conditions. Consequently, the first boundary-initial problem for non-linear reaction-diffusion equation is investigated analytically in the small time-interval by means of integral equations and finite-difference schemes. The approximate solutions are given by means of new absolutely stable explicit finite-difference schemes. The cases of cylindrical, cubical and hexagonal type single crystal growth are considered. Also, in some special cases the effective solutions are obtained. This result is applied to the description of diamond crystal growth.

For the non-linearity of the second order we have introduced some special parameters and obtained new types of the approximate solutions for the pyramidal type crystal growth.

For the case of nanowires (1D nanocrystals) growth we consider the linear reaction-diffusion equation with the appropriate initial-boundary conditions. The approximate solutions are given by means of new absolutely stable explicit finite-difference schemes. In the case of nanoneedles the effective solutions are obtained. The example for growth of germanium nitric nanocrystals is considered.

We hope, that our work will be interesting for chemists and physicists.

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1. Introduction

Let us consider a solid crystal growth accompanied with a chemical reaction. Natural and artificial crystals are formed by the process of crystallization. During this process the solid crystal is formed from a supersaturated solution by means of the chemical reaction. Hence, this is solid-liquid separation at the specific conditions (pressure, temperature, supersaturation etc.) which involves mass transfer from the liquid solution to a pure solid crystalline phase [1-14].

So crystal formation depends on solubility conditions of the solute in the solvent, temperature, pressure, supersaturation [1-14]. When the supersaturation exhausted the solid-liquid system reaches equilibrium and crystallization is completed [1-14]. Sometimes the inverse process could occur. It is usually much easier to dissolve a

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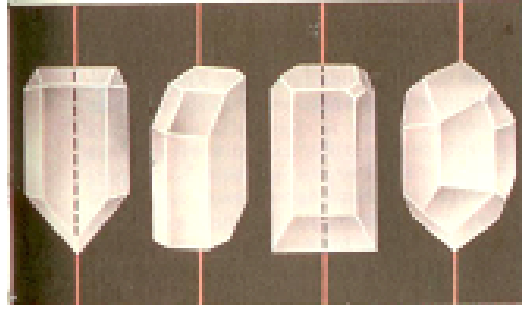


Figure 1. The photo of the vertical quartz crystals (Museum of the Georgian Technical University).

perfect crystal in a solvent, than to grow it again [1,2], but here we will not consider this case.

Crystallization process involves nucleation and crystal growth. At the first step (primary nucleation) the clusters formed from the solvent and in some special conditions cluster becomes are formed nuclei. At this stage the atoms at the cluster are arranged in a periodic structure. This structure is called a crystal structure. After this clusters are growing until supersaturation is exhausted. The growth of clusters is called a secondary crystallization [1-7]. The process of crystallization is natural as well as artificial. The artificial crystals are growing at the definite temperature and pressure at the crystallizer. Some crystals are growing very slow (days and weeks) some—faster (nanocrystals can grow within 5 to 15 minutes [1-9]).

In recent years the growth of nanocrystals for nanodevices becomes very important (nanotubes, nanowires etc). Here we also consider this process. We consider the artificial crystal growth at the crystallizer, for example, quartz reactor [4,5,6,8,9]. The crystallization is accompanied by a lot of complicated processes such as several chemical reactions, evaporation, condensation, heat and energy transfer. Some models of crystal growth are suggested by chemists [1-7, 10,13,14]. These models contain a large number of variables such as free energy, supersaturation, temperature, pressure, velocity of chemical reactions, diffusion coefficients, hydrodynamical characteristics such as viscosity, etc. For the mathematical investigations they need clarification and simplifications.

One of the first mathematical models of the crystallization process, connected with the ice formation (phase transfer model) is known as Stephans problem [22]. In this model the system of two linear diffusion equations for heat transfer with specific boundary conditions is considered.

Mathematical formulation of the diffusion model for the microcrystal growth was first suggested by Itkin [11]. He has considered general Navier Stokes Equation and then modified it to the 1D linear stationary diffusion equation which he solved numerically. The numerical approach is also used in [12], for simplified diffusion equation with the specific boundary conditions.

In our model we take into account only diffusion and velocity of chemical reaction near the surface of the crystal and suggest applying non-linear reaction-diffusion equation with the appropriate boundary conditions. We use the empirical formula of nucleation rate [1,2]. We admit that the direction of the crystal growth is known a priori and is homotopic to the initial surface. We consider a single crystal growth at the given temperature. We admit that in every time-unit certain layer with a constant width (of several nanometer in size) is added to the surface of the crystal.

During this process non-linear reaction-diffusion equation with the appropriate boundary conditions is valid near this area, whilst out of this region ordinary linear diffusion equation is fulfilled. After formation of certain layer the process continues at another region next to the previous layer etc., until supersaturation is exhausted. Then we analyze this model and obtain the approximate solution by means of new finite difference schemes. In some cases we obtain the analytical representation of the solution.

We consider the following process: some highly soluble chemicals are converting into less soluble (solute in the solvent). For the formation of the crystal high initial concentration of solute in the solvent is necessary (supersaturation) and it needs some temperature and pressure for the acceleration of chemical reaction, which precipitate crystal growth near its surface. So we consider diffusion in the solvent and chemical reaction near the surface of the crystal, as a result supersaturation decreases and when it is exhausted the process will stop.

We note that for the construction of some mathematical model it is very important which quantities could be measured. We consider the case when the velocity of the chemical reaction is proportional to a certain degree of supersaturation [1,2] and consider the problem connected with the changes of supersaturation in time.

Hence, in this work we consider the non-linear reaction-diffusion equation with the moving boundary conditions and apply this problem for the description of solid crystals and nanowires growth. For the growth of nanowires we consider the linear model. In this case approximate solutions are also obtained by means of finite-difference schemes. In some particular cases effective solutions are obtained.

Let a single crystal begin to grow from the crystal seed at the definite temperature, pressure and supersaturation. The duration of the growth is the time interval $0 < t < T_0$. We choose the coordinate system $Oxyz$. We consider the single prism type symmetric crystal (or nanowire) growth at the direction of Oz and the plane $Oxyz$ symmetrically (Fig.1). Let us denote by V the area occupied by the crystallizer and by V_t the area occupied by the crystal, V_t changes with the time. The fundament of a crystal is located in the plane Oxy .

This process could be described by the reaction-diffusion equation with moving initial-boundary conditions at the small layer near the crystal, inside certain area V_t^0 (the area V_t^0 contains the crystal). Out of this layer a simple linear diffusion takes place. We admit, that the upper bound of the area V_t^0 is the plane $z = z_0(t)$, where $z_0(t)$ changes in time. Hence, this process is described by the equations

$$\frac{\partial U}{\partial t} = D_0 \Delta U, \quad (x, y, z) \in V - V_t^0, \quad (1^*)$$

$$\frac{\partial U}{\partial t} = D \Delta U - \beta(U, t), \quad (x, y, z) \in V_t^0 - V_t, \quad (\beta \geq 0), \quad z \leq z_0(t), \quad (2^*)$$

$$U(x, y, z, 0) = C_0, \quad U|_{S_1} = 0, \quad U|_{S_2} = 0, \quad 0 < t < T_0,$$

where U is substance supersaturation (unknown function), C_0 is the initial supersaturation, D_0 is the diffusion coefficient in the area $V - V_t^0$, D is the diffusion coefficient in the area $V_t^0 - V_t$, β is a velocity of the chemical reaction, which is generally non-linear function of U and t , S_1 is the boundary of crystallizer V , which

does not changes in time, $S_2(t)$ is the boundary of crystal which depends on time, by $S_0(t)$ we denote the boundary of V_t^0 .

At certain time T_0 this process will stop (when supersaturation is exhausted). The boundary conditions mean that diffusion does not take place at the walls of the crystallizer and inside the crystal. These equations describe a rate of supersaturation distribution in the crystallizer at every moment t .

Some quantities here are defined during the experiment and it is very important what we can measure experimentally. By the experimental results the velocity of crystal growth (or nucleation rate i.e. velocity of chemical reaction) is proportional to some degree of supersaturation U , and is given by the empirical formula [1,2]

$$B(U, t) = \beta(c - c^*)^n, \quad (3^*)$$

where B is the number of nuclei formed per unit volume per unit time (of course it is proportional to the chemical reaction), β is a definite constant (which is calculated from experiments), c is the instantaneous solute concentration, c^* is the concentration of the solute in a saturated solution, $c - c^* = U$ is supersaturation, n is a definite number ranging between 1 and 10, but is generally 2 [1,2].

We consider the following cases

1. $B = \beta U^n(x, y, z, t)$, β is a constant and $V = V_t^0$. Hence, we consider only the equation (2*), the growth at a high temperature in a very short time.

Also, we suggest the following three cases

2. As the formula (3*) is empirical we propose, that $B = \beta z U^n(x, y, t)$ and $U(x, y, z, t) = z U(x, y, t)$, β is a constant. We consider the case, when crystallizer is the infinite tube with the bottom $z = 0$ and at the lateral surface of the crystallizer the supersaturation is zero.

3. In the third case we propose that crystallizer is infinite area and the nucleation rate is $B = \beta U_1^m(z, t) U_2(x, y)$, $U = U_1 \times U_2$, β and m are the given constants.

4. And finally we consider the case of infinite crystallizer and propose $B = \beta U^2(x, y, z, t)$, also $U|_{S_0(t)} = C_1$, where C_1 is the definite constant (the concentration at the boundary of V_t^0 is known).

In chapter 2 the general problem is studied. The problem of existence of the solution in a small time interval is discussed and the approximate solution is obtained by new explicit absolutely stable finite-difference schemes. Besides, we consider the cases 1,2 and 3. For some spacial cases we obtain the effective solutions. This part is theoretical. The example is considered for the linear model.

In chapter 3 the equation (2*) is considered in the case 4. By introducing a new parameter the effective high accurate solutions are obtained. The result is applied to the case of diamond tube growth. The numerical example is given.

In chapter 5 the model of nanowires growth is proposed. We investigated the linear model with the specific boundary conditions. The approximate solution is obtained by means of new explicit finite-difference schemes. For the growth of nanoneedles we have obtained the effective solutions which will be interesting for chemists and physicists. The example of growth of germanium nitric nanowires is considered in the linear case.

2. The growth of prismatic type crystals

Let us introduce the following notations $G = V - V_t$, let G_0 be a projection of G on the plane xoy , G_t is a projection of V_t on the plane xoy , G_v is a projection of V on the plane xoy , G_t^0 is a projection of V_t^0 on the plane xoy , Γ_v is a boundary of G_v , Γ_t is a boundary of G_t , $\Gamma_0 = \Gamma_v + \Gamma_t$ is a boundary of G_0 , Γ_t^0 is a boundary of G_t^0 . We consider the following problems

Problem 1. In the area $Q_T = G \times \{0 < t < T\}$, to find a function U continuous on \bar{Q}_T , having second order derivatives in Q_T , and satisfies the following equation

$$\frac{\partial U}{\partial t} = D\Delta U - \beta U^n(x, y, z, t), \quad (\beta > 0); \quad (1)$$

with the initial and boundary conditions

$$U(x, y, z, 0) = C_0, \quad (2)$$

$$U|_{S_1} = 0, \quad U|_{S_2} = 0; \quad t > 0.$$

(In this case $V_t^0 = V$).

Problem 2. In the area $Q_T = G_0 \times \{0 < t < T\}$, to find a function U continuous on \bar{Q}_T , having second order derivatives in Q_T , and satisfying the following equation

$$\frac{\partial U}{\partial t} = D\Delta U - \beta U^n(x, y, t), \quad (\beta > 0); \quad (3)$$

with the initial and boundary conditions

$$U(x, y, 0) = C_0; \quad U|_{\Gamma_0} = 0; \quad t > 0. \quad (4)$$

Problem 3. In the area $Q_T = G \times \{0 < t < T\}$, to find a function U continuous on \bar{Q}_T , having second order derivatives in Q_T , and satisfying the following equation

$$\frac{\partial U}{\partial t} = D\Delta U - \beta U_1^m(z, t)U_2(x, y), \quad z_1(t) \leq z \leq z_0(t); (\beta > 0); \quad (5)$$

$$\frac{\partial U}{\partial t} = D_0\Delta U; \quad z < z_1(t) \quad \text{or} \quad z > z_0(t); \quad (6)$$

with the initial and boundary conditions

$$\int_{V_t^0} U_1 U_2 dx dy dz|_{t=0} = C_0; \quad U_1|_{z=z_0(t)} = \beta_1(t); \quad U_1|_{z=z_1(t)} = 0,$$

$$z_1(t) \leq z \leq z_0(t); \quad z_1(t) = z_1 + \beta_0(t); \quad z_0(t) = z_1 + h + \beta_0(t);$$

where $\beta_0(t), \beta_1(t)$ are given continuous functions, z_1, h and C_0 are the definite constants, C_0 is the initial supersaturation, which is given at the area V_0^0 .

(The condition (6) means that for $z < z_1(t)$ or $z > z_0(t)$ we have simple diffusion and chemical reaction takes place only at the layer $z_1 + \beta_0(t) \leq z \leq z_1 + h + \beta_0(t)$).

Below we will consider the equation (5). (Here the initial saturation is given in the integral form).

Let us consider this problems one by one.

1. We consider the small time interval $0 < t < t_1$. The equation (1) could be written as

$$\Delta U = \frac{1}{D}\beta U^n + \frac{U - C_0}{Dt}; \quad (7)$$

with the boundary condition

$$U|_{S_1+S_2} = 0.$$

If we suppose that the right hand side of equation (7) is known and consider t as a parameter, we can use a Poissons formula [22,23]

$$U = -\frac{1}{4\pi} \int_{V-V_t} \left\{ \left(\frac{1}{D}\beta U^n + \frac{U - C_0}{Dt} \right) \right\} G(x, y, z, x', y', z') dV', \quad (8)$$

where $dV' = dx'dy'dz'$, $G(x, y, z, x', y', z')$ is a Green's function of Laplacian for the area of integration $V - V_t$. (8) is the integral equation with respect to U . Using Shauder's fixed point principle we conclude [24]:

Conclusion. If

$$C_0 \left(\frac{\beta}{D} + \frac{1}{Dt} \right) |V - V_t| < 4\pi,$$

then there exists the solution U , ($U \leq C_0$) of equation (8) and consequently of Problem 1.

Note. If $U(x, y, z, t) = U(x, y, t)$ and G_0 is a rectangular type area, than $G(x, y, z, x', y', z')$ represents the Weierstrass ζ -function and (6) becomes the integral equation with the Weierstrass kernel [30,31].

2. Now, let us consider Problem 2. By means of the combined method i.e. conformal mapping and finite difference schemes we can obtain the approximate solution of equation (3) for the small time interval which is similar to be equation (7).

At first we map conformally the area G_0 at the rectangle and then use the finite-difference schemes.

Let $z = f(\xi, \eta), z = x + iy$, be the conformal mapping of G_0 at the rectangle D_0 in a new coordinate system $\xi\eta$, then the equation (7) with the boundary condition becomes

$$\Delta U = |f(\xi, \eta)|^2 \frac{1}{D}\beta U^n + |f(\xi, \eta)|^2 \frac{U - C_0}{Dt}; U|_{\Gamma_0} = 0, \quad (9)$$

where t is a parameter, $z = f(w)$, is a conformal mapping of the area G_0 at the rectangle D_0 of the plane w ($w = \xi + i\eta$), $D_0 = \{0 \leq \xi \leq a; 0 \leq \eta \leq b\}$.

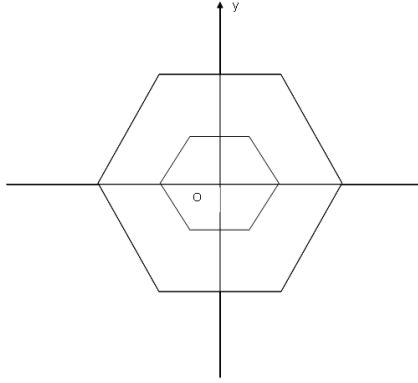


Figure 2. The horizontal cross-section of the hexagonal type crystal.

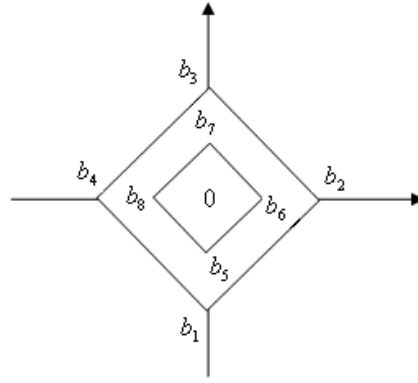


Figure 3. The horizontal cross-section of the hexagonal type crystal.

1. If G_0 is the hexagonal type area (the area among two homotopic concentric hexagons H_1 and H_2) [25,28] (Fig. 2)

$$f'(w) = A \prod_{n=1}^6 \left[\frac{\theta \left(\frac{\ln w - \ln da_n}{2\pi i} \right)}{\theta_1 \left(\frac{\ln w - \ln a_n}{2\pi i} \right)} \right]^{\frac{1}{3}} \cdot \frac{1}{w^2},$$

where $a_n = e^{(2n-1)\frac{\pi i}{n}}$, $n = 1, 2, \dots, 6$, A is a definite constant θ_1 -is the Weierstrass function, $\ln d = b - \frac{\pi i}{2}$.

2. If G_0 is the rectangular type area (the area among two homotopic concentric rectangles R_1 and R_2) (Fig. 3) [25,28]

$$f(w) = B \int_0^{snw} (Z - \alpha_1)^{-\frac{3}{4}} (Z - \alpha_2)^{-\frac{1}{4}} (Z - \alpha_3)^{-\frac{1}{4}} (Z - \alpha_4)^{-\frac{3}{4}} dZ + B_0,$$

where $B; B_0; \alpha_1; \alpha_2; \alpha_3; \alpha_4$ are the definite constants, sn is an elliptic sinus [25].

Now, let us construct the approximate solution by means of the finite-difference schemes for the equation (9) at the area \bar{D}_0 .

The area of integration \bar{D}_0 will be divided by the planes $\xi_i = ih_1, \eta_j = jh_2$, ($i = 0, 1, 2, \dots, M; j = 0, 1, 2, \dots, N$) into cells, where $h_1 = \frac{a}{M}$, $h_2 = \frac{b}{N}$. Consequently, for the area \bar{D}_0 we introduce the following grids $\bar{\omega}_h = \{\xi_i = ih_1, \eta_j = jh_2, i = 0, 1, \dots, M, j = 0, 1, \dots, N\}$, For net functions and their difference derivatives we introduce the following notation

$$U_{\xi_1} = \frac{1}{h_1}(U(\xi + h_1, \eta) - U(\xi, \eta)), \quad U_{\eta_2} = \frac{1}{h_2}(U(\xi, \eta + h_2) - U(\xi, \eta)),$$

$$U_{\bar{\xi}_1} = \frac{1}{h_1}(U(\xi, \eta) - U(\xi - h_1, \eta)), \quad U_{\bar{\xi}_2} = \frac{1}{h_2}(U(\xi, \eta) - U(\xi, \eta - h_2)),$$

$$\Delta_2 U = U_{\eta_2} = \frac{1}{2}(U_{\eta_2} + U_{\bar{\eta}_2}), \quad \Delta_{11} U = U_{\xi\bar{\xi}}, \quad \Delta_{22} U = U_{\eta\bar{\eta}}.$$

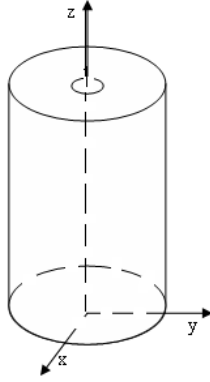


Figure 4. Cylindrical crystallizer of the radii $6\mu\text{m}$ with the crystal of radii $3\mu\text{m}$ inside.

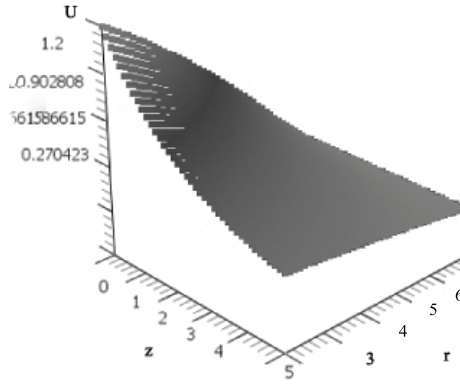


Figure 5. The axi-symmetric case, $D = 0.13\mu\text{m}^2/\text{s}$; $r^2 = x^2 + y^2$; $C_0 = 1.17\text{pkL}$; $\beta = 0.43\text{pkL}/\text{s}$; $t = 3\text{sec}$.

For the approximation of problem (9) we introduce the following explicit symmetric finite difference schemes

$$-\sigma\tau^2\Delta_{11}\frac{U^{k+1} - 2U^k + U^{k-1}}{\tau^2} = U_{x_1\bar{x}_1}^k + U_{x_2\bar{x}_2}^k + (g)_{ij}^k, \quad (10)$$

$$\phi_{ij} = \left\{ \frac{U_{i-1,j}^{k+1} - 2U_{ij}^{k+1} + U_{i+1,j}^{k+1}}{h_1^2} - 2\frac{U_{i-1,j}^k - 2U_{ij}^k + U_{i+1,j}^k}{h_1^2} + \frac{U_{i-1,j}^{k-1} - 2U_{ij}^{k-1} + U_{i+1,j}^{k-1}}{h_1^2} \right\},$$

$$F_{ij} = -\frac{2\sigma}{h_1^2}[U_{i-1,j}^k - U_{ij}^k + U_{i+1,j}^k] + \frac{1}{h_1^2}(U_{i-1,j}^k - 2U_{ij}^k + U_{i+1,j}^k)$$

$$+ \frac{\sigma}{h_1^2}(U_{i-1,j}^{k-1} - 2U_{ij}^{k-1} + U_{i+1,j}^{k-1}) + \frac{1}{h_1^2}(U_{i,j-1}^k - 2U_{ij}^k + U_{i,j+1}^k) + (g)_{ij}^k, \quad (11)$$

where σ is a definite parameter,

$$g = |f(\xi, \eta)|^2 \frac{1}{D}\beta U^n + |f(\xi, \eta)|^2 \frac{U - C_0}{Dt}.$$

The accuracy of schemes (10), (11) is $O(\tau, h^2)$ and is proved similar to [26, 27].

Example 1. Some crystals could be modeled as cylindrical body and we can consider the growth of cylinder at the cylindrical crystallizer (Fig. 4). In this case we obtain the initial-boundary value problem for axi-symmetric reaction-diffusion equation. In case of $n = 1$ the numerical result is obtained using C^{++} by means of schemes (10),(11). The graph of supersaturation distribution for some parameters is given below (Fig. 5).

Analogous schemes were used in [32]. The case of $n = 2$ is considered in Chapter 3. The numerical analysis in case of $n > 2$ is in preparation.

3. Let us consider Problem 3 for the layer $z_1(t) \leq z \leq z_0(t)$. For the functions

U_1 and U_2 we have to solve the following boundary value problems

Problem 3a. In the area $Q_T^1 = \{0 < z < z_T\} \times \{0 < t < T\}$, to find a function U_1 continuous on \bar{Q}_T^2 , having second order derivatives, satisfying the following equation

$$\frac{\partial U_1}{\partial t} = D\Delta U_1 - \beta U_1^m(z, t) + \beta_2 U_1(z, t), \quad (\beta > 0; m \geq 1), \quad (12)$$

with initial-boundary conditions

$$U_1|_{z=z_1+h+\beta_0(t)} = \beta_1(t), \quad U_1|_{z=z_1+\beta_0(t)} = 0, \quad (13)$$

$$z_1 + \beta_0(t) \leq z \leq z_1 + h + \beta_0(t);$$

where $\beta_2 > 0$ is some constant.

For small time interval $0 < t < t_1$ we suppose $\beta_0(t) = \beta t$, $\beta_0, \beta_1(t)$ are the given constants. From (12), (13) we obtain

$$(U_1)'' = \frac{1}{D}\beta U_1^m + \frac{U_1 - \beta_1}{Dt} - \frac{\beta_2 U_1}{Dt}; \quad (14)$$

The equation (14) is the ordinary differential equation. The solution of this equation in an implicit form is

$$z = \sqrt{2} \int_0^{U_1} \frac{dy}{\sqrt{\frac{\beta}{D(m+1)}y^{m+1} + \frac{(1-\beta_2)y^2}{2Dt} - \frac{\beta_1 y}{Dt}}} + z_1 + \beta_0 t. \quad (15)$$

In case of $m = 2$, (15) represents an elliptic integral and consequently U_1 is an elliptic function.

Problem 3b. In the area G_v to find a function $U_2 > 0$ continuous on \bar{G}_v vanishing at the boundary G_v , having second order derivatives and satisfying the following equation

$$\Delta U_2 - \frac{\beta_2}{D} U_2(x, y) = 0, \quad (16)$$

where β_2 is the definite constant.

Also for Problems 3a and 3b the following condition is fulfilled

$$\int_{V_t^0} U_1 U_2 dx dy dz|_{t=0} = C_0,$$

The Problem 3b is a well-known Helmholtz Problem [22,23].

In the sequel we will consider the solutions of (16) of the form

$$U_2 = \cos k(a|x| + b|y| - a_0); \quad \beta_2 = -\beta_2^*; \quad \beta_2^* > 0, \quad (17)$$

where $\beta_2^* = 4Dk^2; k = (\pi)/(\alpha a_0 - a_0)$, $2\alpha a_0$ ($\alpha > 1, a_0 > 0$) is the diameter of the crystallizer, and

$$U_2 = e^{-a|x|-b|y|-d}, \beta_2 \geq 0, \tag{18}$$

where $\beta_2 = D(a^2 + b^2), a, b, d > 0$, are certain constants satisfying the condition $\beta_2 = D(a^2 + b^2)$.

This solutions (18) and (19) are constants at the surfaces $a|x| + b|y| = a_0; a_0 > 0, a_0$ is a constant.

Below the example is given in the linear case.

The case $m = 1$. In the case of $m = 1$ the solution of Problem 3a will be obtained by the separation of variables and is given by [22,23]

$$U_1 = \beta_1(e^{h\frac{\beta_0}{D}} - e^{\frac{\beta_0}{D}(z_1+h+\beta_0t-z)})e^{-\beta_3^*t}, \quad z_1 + \beta_0t \leq z \leq z_1 + h + \beta_0t,$$

where $\beta_1(t) = \beta_1^*e^{-\beta_3^*t}, \beta_1^* = \frac{\beta_1}{e^{h\frac{\beta_0}{D}} - 1}, \beta_1$ and β_3^* are certain constants.

Let us consider the growth of the crystal of rectangular cross section in the direction of Oz (Fig. 6). For this case Γ_t is a rectangle $|x| + |y| = a_0; a_0 > 0$ (the cross-section of a crystal by planes parallel to xOy does not changes in time, it changes only in the direction of Oz). Taking into account (17) the solution of Problem 3 at the layer $z_1 + \beta_0t \leq z \leq z_1 + h + \beta_0t$ will be given by

$$U = \phi_1 \cos k(|x| + |y| - a_0), \quad |x| + |y| \leq a_0; z_1 + \beta_0t \leq z \leq z_1 + h + \beta_0t, \tag{19}$$

$$U = \phi_2 \cos k(|x| + |y| - a_0), \quad |x| + |y| > a_0; z_1 + \beta_0t \leq z \leq z_1 + h + \beta_0t,$$

where

$$\phi_1 = \beta_1(e^{h\frac{\beta_0}{D}} - e^{\frac{\beta_0}{D}(z_1+h+\beta_0t-z)})e^{-\beta_3t}, \quad \phi_2 = \beta_1(e^{h\frac{\beta_0}{D}} - e^{\frac{\beta_0}{D}(z_1+h+\beta_0t-z)})e^{-\beta_2^*t},$$

$$\int_{V_t^0} U dx dy dz \Big|_{t=0} = C_0,$$

$\beta_3 = \beta + \beta_2^*, C_0$ is the initial supersaturation.

It is obvious that the function U is discontinuous at the surface $|x| + |y| = a_0; z_1 + \beta_0t \leq z \leq z_1 + h + \beta_0t$.

Note 1. We note that as we consider the ideal case, the layer where the reaction takes place is not exactly bounded by horizontal planes, but by some curves which are approximately horizontal.

Note 2. At the area $|x| + |y| > a_0; 0 \leq z < z_1 + \beta_0t$, the growth process is completed and theoretically it is possible that here we have simple diffusion. In this case the solution at this area is represented in the form

$$U = \beta_1 e^{-\beta_2^*t} (e^{\frac{\beta_0}{D}(z_1+h+\beta_0t-z)} - e^{h\frac{\beta_0}{D}}) \sin 2k(|x| + |y| - a_0),$$

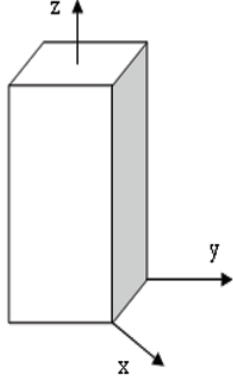


Figure 6. prismatic type crystal with a rectangular cross-section of diameter $10^3\mu m$.

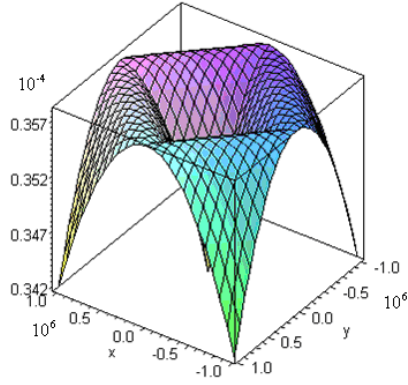


Figure 7. $z = \beta_0 t + z_0$; $z_0 = 3$; $\beta_3 = 0.01$; $t = 100sec$.

and for $z > z_1 + h + \beta_0 t$, in the form

$$U = \beta_1 e^{-\beta_2^* t} (e^{h \frac{\beta_0}{D}} - e^{\frac{\beta_0}{D}(z_1 + h + \beta_0 t - z)}) \cos k(|x| + |y| - a_0).$$

Example 1.

Let us consider the growth of synthetic diamond by chemical vapor deposition technique (CVD method).

CVD method involves pyrolysis of hydrocarbon gases in the chamber at the relatively low temperature (about 800^0C) and pressure (about $27kPa$) [7,33,34].

We consider a growth of a single crystal diamond on a diamond seed in a chamber by means of gases methan (carbon source) and hydrogen. This method was successfully developed in the middle of the XX-th century [7,33,34,35] and can produce single crystals several millimeter in size. B. Deriagin and D. Fedoseev has grown diamond wire about of $10^3\mu m$ in diameter [7]. Growth rate was about $1/4\mu m$ in an hour, consequently $\beta_0 = (1/144) \times 10^{-2}\mu m/sec = 7 \times 10^{-2}nm/sec$.

We have used the following data: the diffusion coefficient of Methan at the pressure 1 bar is $2 \times 10^{-1}\mu m^2/s$ [www.engineeringtoolbox.com.diffusion-coefficients]. Consequently, at the temperature about 800^0C and pressure $27kPa$ it will be about $D = 2 \times 10^{-14}\mu m^2/s$, it is about 6×10^{-2} molecules in nm^2/s . The density of diamond is about $3.5 \times 10^{-6}\mu g/\mu m^3$ [35]. The volume of growth crystal in 1 sec will be $v = (1/144) \times 10^{-4}\mu m^3$, the mass $M = (1/4) \times 10^{-5}\mu g$.

About 10 times more carbon allotrops are necessary for the growth of some unit mass of diamond [7,33,34,35]. Consequently, we suppose that the initial saturataion near the initial seed will be $C_0 = (1/4) \times 10^{-4}\mu g = (1/4) \times 10^5 mol$. We will consider the growth only in the direction Oz and suppose $a_0 = (10^6/2)nm$; $a = b = 1$; $z_1 = 0$, $\frac{\beta_0}{D} \approx 7/6$.

At the area $|x| + |y| \leq 10^6/2$; $z_1 + \beta_0 t \leq z \leq z_1 + h + \beta_0 t$ by formula (19) we have

$$U = (C_0 k^2) / (8h(\pi - 2)) (e^{h \frac{\beta_0}{D}} - e^{\frac{\beta_0}{D}(z_1 + h + \beta_0 t - z)}) e^{-\beta_3 t} \cos k(|x| + |y| - a_0), \quad (20)$$

$$C_0 = \int_{V_0^0} U dx dy dz \approx (8\beta_1 h(\pi - 2)) / k^2.$$

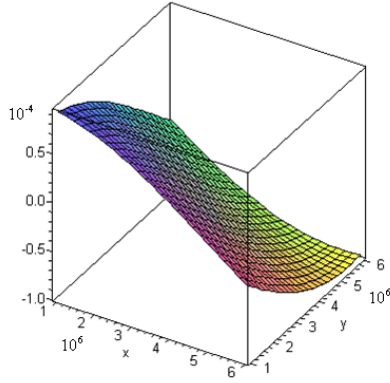


Figure 8. $z = \beta_0 t + z_0$; $z_0 = 3$; $\beta_3 = 0.01$; $t = 100$.

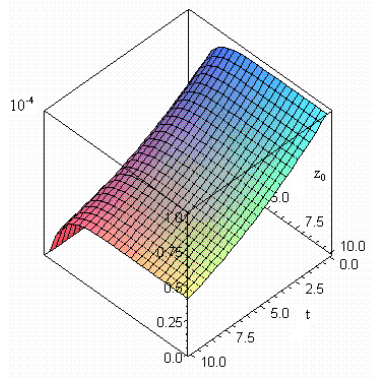


Figure 9. $z = \beta_0 t + z_0$; $\beta_3 = 0.1$; $x = y = 0.13 \times 10^6$.

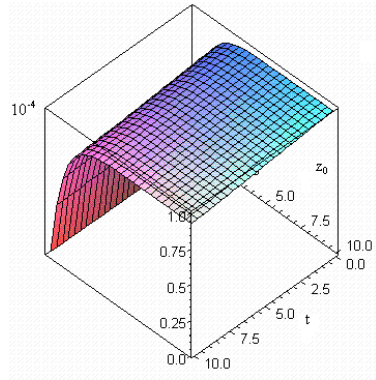


Figure 10. $z = \beta_0 t + z_0$; $\beta_3 = 0.01$; $x = y = 0.13 \times 10^6$.

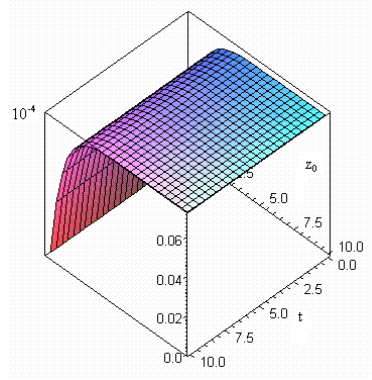


Figure 11. $z = \beta_0 t + z_0$; $\beta_2^* = 10^{-8}$; $x = y = 1.5 \times 10^6$.

In Figures 7,8,9,10,11 the graphs of (20) are given for the different parameters (the graphs are constructed by using Maple).

Note 3. Synthetic diamond is the hardest material known. Some synthetic nanocrystalline diamonds (hyperdiamonds) are harder than any known natural diamond [36].

Note 4. The shape of prismatic type has some quartz and insulin crystals,also germanium nanocrystals [9].

3. The growth of pyramidal type crystals

Here we consider the case, when the size of crystal is rather small in comparison with the size of crystallizer and consider the equation (2*) for the small time interval $0 < t < t_1$ in case of $n = 2$. Also, we suppose, that the shape of the initial seed is a pyramidal $V_0 : a|x| + b|y| + c|z| \leq \epsilon; \epsilon, a, b, c > 0$ (Fig. 12). Hence, we consider the following equation

$$\Delta U = \frac{1}{D} \beta U^2 + \frac{U - C_0}{Dt}; \tag{21}$$

with the boundary conditions

$$U|_{S_2(0)} = 0, \quad U|_S = C_0,$$

where C_0 is the initial supersaturation, S is a certain surface $a|x| + b|y| + c|z| = \epsilon_0$; $\epsilon < \epsilon_0$, the constant ϵ_0 will be defined below.

We seek the symmetric solutions of (21) in the form

$$U = R \cos \psi - C^*, \quad (22)$$

where R is some constant and $\psi(x, y, z)$ is a sufficiently small unknown function for which ψ^3 is negligible.

According to (22) equation (21) becomes

$$\begin{aligned} & -R \sin \psi \Delta \psi - R \cos \psi \left\{ \left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial \psi}{\partial y} \right)^2 + \left(\frac{\partial \psi}{\partial z} \right)^2 \right\} \\ & = \frac{\beta}{D} (R \cos \psi - C^*)^2 + \frac{1}{Dt} (R \cos \psi - C^*) - \frac{C_0}{Dt}; \end{aligned} \quad (23)$$

The equation (23) is the non-linear partial differential equation with respect to $\psi(x, y, z)$. Taking into account that ψ^3 is sufficiently small and putting into (20) the formulas

$$\sin \psi \approx \psi, \quad \cos \psi \approx 1 - \frac{\psi^2}{2},$$

we obtain the equation

$$\begin{aligned} & -R \psi \Delta \psi - R \left(1 - \frac{\psi^2}{2}\right) \left\{ \left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial \psi}{\partial y} \right)^2 + \left(\frac{\partial \psi}{\partial z} \right)^2 \right\} \\ & = \frac{\beta}{D} ((R - C^*)^2 - R(R - C^*)\psi^2) + \frac{1}{Dt} (R - C^*) - \frac{R}{2Dt} \psi^2 - \frac{C_0}{Dt}; \end{aligned} \quad (24)$$

For equation (24) we will solve the following problem

Problem 4. In the area G_0 to find symmetric continuous function ψ of the class $O(e^{-4})$, having second order derivatives and satisfying the equation (21).

By direct verification we obtain that the solution of Problem 4 is given by the formula

$$\psi = e^{-a|x| - b|y| - c|z| - d}, \quad (25)$$

where the constants a, b, c, d satisfy the following conditions

$$\begin{aligned} a^2 + b^2 + c^2 &= \frac{1}{4Dt} \sqrt{1 + 4\beta C_0 t} \\ R - C^* &= \frac{-1 + \sqrt{1 + 4\beta C_0 t}}{2\beta t}. \end{aligned} \quad (26)$$

and d is the constant chosen for the desired accuracy in such a way, that e^{-3d} is negligible (for example for $d = 4$, $e^{-12} \approx 6 \times 10^{-6}$).

It is clear from (25) that ψ belongs to the class $O(e^{-4})$, and

$$|\psi| \leq e^{-d}. \tag{27}$$

The function given by the formulae (25),(26) will be the solution of the equation (21) if we ignore the terms

$$\frac{R\psi^4(a^2 + b^2 + c^2)}{2}; -\frac{\beta R^2\psi^4}{4D}.$$

Hence, if d is chosen accordingly and ψ belongs to the class $O(e^{-d})$, then we can conclude, that the function given by (25) is the effective solution of equation (21).

According to (25) and conditions (26),(27) we have the following accuracy

$$\left| R\psi\Delta\psi + R\left(1 - \frac{\psi^2}{2}\right) \left\{ \left(\frac{\partial\psi}{\partial x}\right)^2 + \left(\frac{\partial\psi}{\partial y}\right)^2 + \left(\frac{\partial\psi}{\partial z}\right)^2 \right\} + \frac{\beta}{D}(R\cos\psi - C^*)^2 + \frac{1}{Dt}(R\cos\psi - C^*) - \frac{C_0}{Dt} \right| = \psi^4 R \left| \frac{(a^2 + b^2 + c^2)}{2} - \frac{\beta R}{4D} \right|.$$

Consequently the solution of (21) will be given by

$$U = R\cos e^{-a|x|-b|y|-c|z|-d} - C^*, \tag{28}$$

where the constants $R, C^*, d, a, b, c > 0$ satisfy the condition (26), $\epsilon_0 = 8; C_0 = R - C^*; C^* = R\cos e^{-\epsilon-d}$.

Note 1. The first order derivatives of the function (28) has discontinuities at the planes $x = 0; y = 0; z = 0$, but their squares are continuous (as the limits of first derivatives), besides the second order derivatives exist at these planes and equation (21) holds.

Also it is obvious from (21) that, if t tends to zero, U tends to $R - C^*$.

Conclusion. There exist the solutions of the equation (21) of the class $O(e^{-4})$, they are given by formula (28) and their modulus satisfies the inequality

$$|\Psi| \leq Re^{-d},$$

where d is the constant for which e^{-3d} is negligible.

Below graph of U is plotted using "Maple"(Fig. 13)

Note 2. The shape of pyramidal type has some quartz crystals and germanium nanocrystals [9]. As a rule at the end of the growth prismatic type crystals form pyramidal shaped structures.

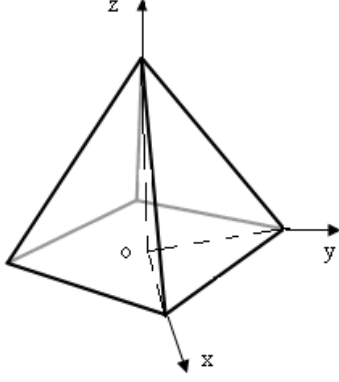


Figure 12. The image of tetrahedral crystal.

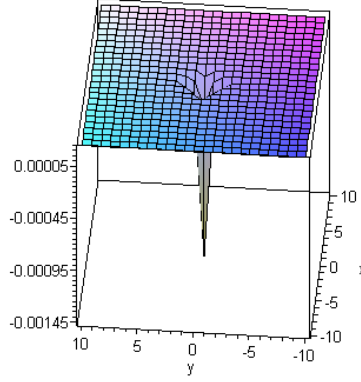


Figure 13. $R = 10$; $z = 1.2$; $\epsilon = 1$; $C_0 = 2 \times 10^{-4}$.

4. The growth of nanowires

Now let us consider the problem connected with the 1D crystal (nanowires) growth (Fig. 4). Let us consider the ideal model: let us three branches of crystal growth in the direction of lines $(x = y; z = 0)$, $(x = z; y = 0)$ and $(y = z; x = 0)$ at the constant speed β (Fig. 14, Fig. 15) (we interpreted branches of the crystal as straight lines). Suppose that reaction-diffusion equation is linear. We consider this equation in the first octant of $oxyz$ plane with the specific boundary conditions i.e. along the lines $(x = y; z = 0)$, $(x = z; y = 0)$ and $(y = z; x = 0)$ boundary function becomes zero, and the reaction takes place in the small area $\{0 < x < a\} \times \{0 < y < a\} \times \{0 < z < a\}$.

Problem 5. In the area $Q_T = \{0 < x < a\} \times \{0 < y < a\} \times \{0 < z < a\} \times \{0 < t < T\}$, to find a function U continuous on \bar{Q}_T , having second order derivatives in Q_T , satisfying the following equation

$$\frac{\partial U}{\partial t} = D\Delta U - \beta U, \quad (\beta = \text{const} > 0); \quad (29)$$

with the initial and boundary conditions

$$U(x, y, z, 0) = C_0, \quad (30)$$

$$U|_{x=0} = (y - a) \left\{ e^{-\frac{\beta_0}{D}(z - \beta_0 t)} - e^{-\frac{\beta_0}{D}(a - \beta_0 t)} \right\} - (z - a) \left\{ e^{-\frac{\beta_0}{D}(y - \beta_0 t)} - e^{-\frac{\beta_0}{D}(a - \beta_0 t)} \right\} \equiv f_1;$$

$$U|_{y=0} = (z - a) \left\{ e^{-\frac{\beta_0}{D}(x - \beta_0 t)} - e^{-\frac{\beta_0}{D}(a - \beta_0 t)} \right\} - (x - a) \left\{ e^{-\frac{\beta_0}{D}(z - \beta_0 t)} - e^{-\frac{\beta_0}{D}(a - \beta_0 t)} \right\} \equiv f_2;$$

$$U|_{z=0} = (x - a) \left\{ e^{-\frac{\beta_0}{D}(y-\beta_0 t)} - e^{-\frac{\beta_0}{D}(a-\beta_0 t)} \right\} \\ - (y - a) \left\{ e^{-\frac{\beta_0}{D}(x-\beta_0 t)} - e^{-\frac{\beta_0}{D}(a-\beta_0 t)} \right\} \equiv f_3;$$

$$t > 0; x > 0; y > 0;$$

where a, β and β_0 are definite constants.

In this case the approximate solution of (29) (30) will be given by explicit finite-difference schemes [26,27].

We suppose $a = 1$ and the domain of integration Q_T will be divided into elementary cells by planes $x_i = ih, y_j = jh, z_m = mh, t_n = n\tau, (i, j, m = 0, 1, 2, \dots, M; n = 0, 1, \dots, M_0)$, where $h = \frac{1}{M}; \tau = \frac{T}{M_0}; \bar{\omega}_\tau$ is a net with the step $\tau = \frac{T}{M_0}$ and

$$\bar{\omega}_h = \{x_i = ih_1, y_j = jh_2, z_m = mh; i, j, m = 0, 1, \dots, M\},$$

$$\frac{u^{n+k} - u^{n+k-2}}{2\tau} = 1.5\{\Delta_{kk}(u^{n+k} - u^{n+k-2})\} + \sum_{i=1}^3 \Delta_{ii}u^{n+k-2} - 0.5\beta(u^{n+k} - u^{n+k-2}),$$

$$\frac{u^{n+\frac{k}{3}} - u^{n+\frac{k-1}{3}}}{\frac{1}{3}\tau} = 1.5\{\Delta_{kk}(u^{n+\frac{k}{3}} - u^{n+\frac{k-1}{3}})\} + \sum_{i=1}^3 \Delta_{ii}u^{n+k-2} - 0.5\beta(u^{n+k} - u^{n+k-2}),$$

where $k = 1, 2, 3; (x_i, y_j, z_m, t_n) \in \bar{\omega}_h \times \bar{\omega}_\tau,$

$$\Delta_{11}u = u_{x\bar{x}} = \frac{1}{h^2} [u(x + h, y, z, t_n) - 2u(x, y, z, t_n) + u(x - h, y, z, t_n)] \approx D \frac{\partial^2 u}{\partial x^2},$$

$$\Delta_{22}u = u_{y,\bar{y}} = \frac{1}{h^2} [u(x, y + h, z, t_n) - 2u(x, y, z, t_n) + u(x, y - h, z, t_n)] \approx D \frac{\partial^2 u}{\partial y^2},$$

$$\Delta_{33}u = u_{z\bar{z}} = \frac{1}{h^2} [u(x, y, z + h, t_n) - 2u(x, y, z, t_n) + u(x, y, z - h, t_n)] \approx D \frac{\partial^2 u}{\partial z^2},$$

The initial and boundary conditions take the form

$$U(x_i, y_j, z_m, 0) = C_0; U(0, y_j, z_m, t_n) = f_1(y_j, z_m, t_n);$$

$$U(x_i, 0, z_m, t_n) = f_2(x_i, z_m, t_n); U(x_i, y_j, 0, t_n) = f_3(x_i, y_j, t_n).$$

These schemes are absolutely stable economical schemes having complete approximation [26,27].

In some cases we can obtain the effective solutions. Let us consider the growth of vertical nanoneedles (the chemical process is considered in [8,9], the diameter of nanoneedle is about 1nm.) Consider the following problem

Problem 6. In the area $Q_T^0 = \{-a < x < a\} \times \{-a < y < a\} \times \{0 < z < h\} \times \{0 < t < T\}$, to find a function U continuous on \bar{Q}_T^0 , having second order derivatives in Q_T^0 , satisfying the following equation

$$\frac{\partial U}{\partial t} = D\Delta U, \quad z < z_1 + \beta_0 t, \quad (31)$$

$$\frac{\partial U}{\partial t} = D\Delta U - \beta U, \quad z_1 + \beta_0 t < z < z_1 + h + \beta_0 t,$$

and the initial-boundary conditions

$$U_1|_{z=z_1+h+\beta_0 t} = \beta_1(t), \quad U_1|_{z=z_1+\beta_0 t} = 0,$$

$$U|_{|x|+|y|=a_0} = 0; \quad z \leq z_1 + \beta_0 t; \quad \int_{\bar{Q}_T^0} U dx dy dz|_{t=0} = C_0, \quad (32)$$

where $\beta_1(t) = \beta_1^* e^{-\beta_3^* t}$, $\beta_1^* = \frac{\beta_1}{e^{h\frac{\beta_0}{D}} - 1}$, $\beta_1, \beta, \beta_0, \beta_1, \beta_3^* > 0$ are definite constants C_0 is the initial supersaturation, $2a_0$ is the diameter of the, nanoneedle.

Using formula (18) from chapter 2 by direct verification we obtain that the solution of Problem 6 will be given by

$$U = e^{-b|x|-b|y|-d} \phi_1, \quad |x| + |y| \leq a_0, \quad z_1 + \beta_0 t \leq z \leq z_1 + h + \beta_0 t, \quad (33)$$

$$U = \phi_2 \cos k(|x| + |y| - a_0), \quad |x| + |y| > a_0, \quad z_1 + \beta_0 t \leq z \leq z_1 + h + \beta_0 t,$$

$$U = \beta_1 e^{-k_0 t} (e^{\frac{\beta_0}{D}(z_1+h+\beta_0 t-z)} - e^{h\frac{\beta_0}{D}}) \sin 2k(|x| + |y| - a_0), \quad z < z_1 + \beta_0 t,$$

where $k, k_0 > 0$ are the certain constants, $k = \pi/2(a - a_0)$, $k_0 = 4Dk^2$, $\beta_3 = \beta - \beta_2$, $\beta_2 = D(a^2 + b^2)$,

$$\phi_1 = \beta_1 (e^{h\frac{\beta_0}{D}} - e^{\frac{\beta_0}{D}(z_1+h+\beta_0 t-z)}) e^{-\beta_3 t},$$

$$\phi_2 = \beta_1 (e^{h\frac{\beta_0}{D}} - e^{\frac{\beta_0}{D}(z_1+h+\beta_0 t-z)}) e^{-k_0 t}.$$

Now, let us consider the growth of vertical nanoneedles periodically distributed at the plane Oxy with the period p ; $p > 0$. Suppose, that nanoneedles are straight lines and the crystallizer is an infinite area (as the size of nanoneedle is rather small

in comparison with the size of crystallizer). In this case the nucleation rate and growth rate are equal.

We consider the following problem

Problem 7. In the area $Q_T^0 = z > 0 \times \{0 < t < T\}$, to find a function U continuous on \bar{Q}_T^0 , having second order derivatives in Q_T^0 , satisfying the following equation

$$\frac{\partial U}{\partial t} = D\Delta U, \quad (34)$$

and the initial-boundary conditions

$$U|_{x=pn, y=pm} = 0; m, n = 0, \pm 1, \pm 2, \dots; z \leq \beta t;$$

$$\int_{|x|+|y| \leq p/4} \int_0^h U dx dy dz = C_0,$$

where h is a certain constant.

By direct verification we obtain that the solution of (34) will be given by

$$U = A|U_0(x, y)|(e^{-\frac{\beta}{D}(z-\beta t)} - 1), z \leq \beta t,$$

$$U = A(|U_0(x, y)| + C^*)(1 - e^{-\frac{\beta}{D}(z-\beta t)}), z > \beta t,$$

$A, C^*, C^* > 0$ are the definite constants, $U_0(x, y)$ is the doubly-periodic harmonic function with zeros at the points $x = pn; y = pm; m, n = 0, \pm 1, \pm 2, \dots$

Note 1. The Problem 7 is discussed in more detailed in the paper of the authors which is prepared for the publication.

Example 2.

Let us consider the growth of Ge_3N_4 nanowires by chemical vapor deposition technique (CVD method). This method was developed at the Chemical Laboratory of Georgian Technical University [8,9]. The nanowire of $1\mu m$ was produced in 10 minutes at the Quartz crystallizer at the temperature about $520^\circ C$ and pressure about $10Pa$ in the vapor of hydrazine diluted with 3% mol water. The nucleation and mass transfer was performed through synthesis of volatile GeO molecules, their re-deposition and formation of GeO clusters which served as surfaces where Ge_3N_4 nuclei was synthesized [9].

We have used the following data: the diffusion coefficient of Nitrogen at the pressure 1 atmosphere is $0.53cm^2/s$

[www.medical-dictionary.thefreedictionary.com/diffusion+coefficients]. Consequently, at the temperature about $520^\circ C$ and pressure $10Pa$ it will be about $D = 10^{-7}nm^2/s$ (is about 2×10^5 molecules in nm^2/s). The growth rate is about $(1/6)10^2 nm/s$, it is about $2 \times 10^5/3$ nitrid atoms (due to the nucleation rate), consequently in 10 seconds about $2/3 \times 10^6$ molecules are formed.

We suppose, that the initial supersaturataion near the initial seed will be $C_0 = 4 \times 10^7$ molecules. We will consider the growth only in the direction Oz and suppose

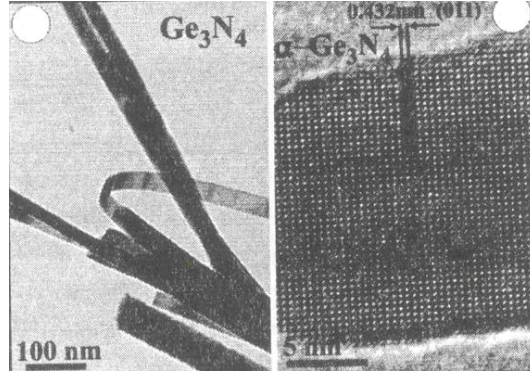


Figure 14. The image of germanium nitride nanowires (copied from [9]).

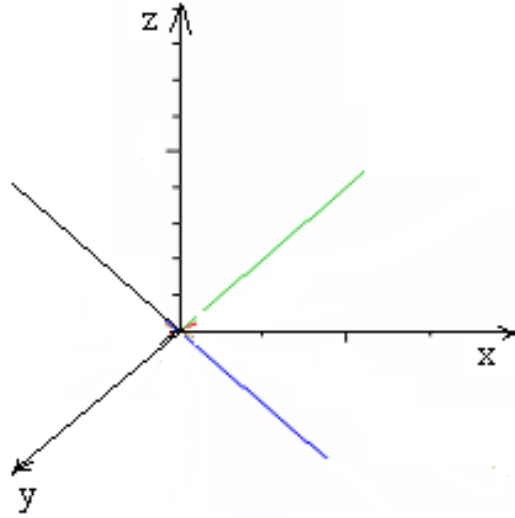


Figure 15. The artificial scheme of nanowires (lines $(x = y; z = 0)$, $(x = z; y = 0)$ and $(y = z; x = 0)$).

$a_0 = 1$; $a = b = 1$; $h = 4nm$; $z_1 = 0$; $\beta_0 = \frac{2}{3}10^5 mol/s$, $\frac{\beta_0}{D} \approx 1/3$, $\beta_2 = 2D$ and $\beta = 2D + \beta_3$; $\beta_3 > 0$.

At the layer $|x| + |y| < a_0$; $z_1 + \beta_0 t \leq z \leq z_1 + h + \beta_0 t$ by formula (33) we have

$$U = \frac{C_0}{(1 - e^{-a_0} - a_0 e^{-a_0})(h + \frac{D}{\beta_0}(e^{-h\frac{\beta_0}{D}} - 1))} e^{-|x|-|y|} (1 - e^{(\beta_0 t - z)\frac{\beta_0}{D}}) e^{-\beta_3 t}. \quad (35)$$

Below, the graphs of (35) are given for the different parameters (the graphs are constructed by using Maple, Figures 16,17,18,19)

Conclusion. We obtain the relationship between supersaturation, diffusion coefficient and the chemical reaction of the crystallization process.

Note 2. By the equation (29) the heat conduction at the homogeneous crystal is also described [37].

Note 3. In the examples some quantities such as diffusion coefficients contain

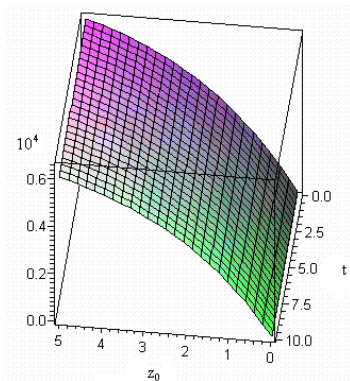


Figure 16. $z = \beta_0 t + z_0$; $\beta_3 = 0.01$;
 $x = y = 0.25$.

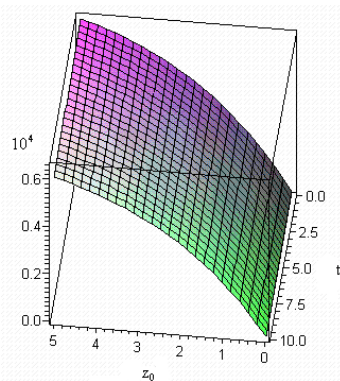


Figure 17. $z = \beta_0 t + z_0$; $\beta_3 = 0.01$;
 $x = y = 0.1$.

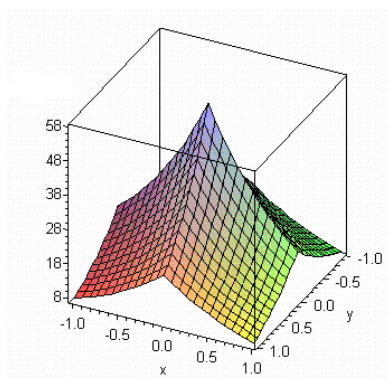


Figure 18. $z = \beta_0 t + z_0$; $\beta_3 = 0.01$;
 $z_0 = 0.2$; $t = 10$.

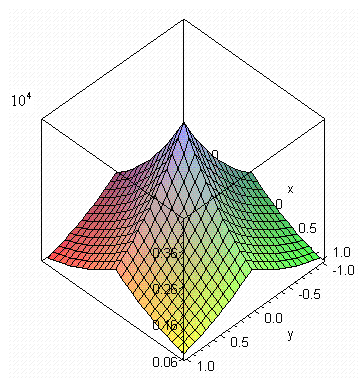


Figure 19. $z = \beta_0 t + z_0$; $\beta_3 = 0.01$;
 $z_0 = 2$; $t = 10$.

errors of measurement.

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