

**MATHEMATICAL MODEL OF TECHNOLOGICAL PROCESS
OF MANUFACTURING THIN FILMS TAKING INTO
ACCOUNT THEIR ANISOTROPY AND HETEROGENEITY**

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Abstract

The problem of diffusion in the fabrication process of thin-film structures with crystal anisotropy and heterogeneity is considered. Two boundary value problems A and B are posed with respect to impurity atoms in the crystal bulk. Boundary value problem A describes the process of diffusion with an open window for atoms in the gas phase (to penetrate through it into the crystal), and boundary value problem B is a diffusion process with a closed window (diffusant atoms are redistributed in the crystal during high-temperature oxidation). These boundary value problems are solved by the Green's function method. Using the methods of tensor analysis and Riemannian geometry, the modified Green's functions for boundary value problems A and B are determined in the form of finite analytic functions. Solutions are found as finite integral expressions, with the help of which the diffusant concentrations are calculated at an arbitrary point for various moments of time. The cases of thick (when the crystal thickness exceeds the diffusion length) and thin (when it is less than the diffusion length) crystals are considered. The Green's function for thin crystals is plotted as infinite coinciding lines.

Increase of demands to accuracy of calculation and analysis methods of semiconductor structures applied during designing of devices on these structures requires development of more perfect methods of mathematical simulation. Very important semiconductor structures for development of various devices of micro- and nanoelectronics are thin films and that is why it is of great interest to create the mathematical model of technological processes of their fabrication. Diffusion is one of the most important technological processes determining the thin film based semiconductor devices operation.

This paper is devoted to 3D model of diffusion process during fabrication of a thin film semiconductor crystal structure with anisotropy and heterogeneity. The 3D consideration of the diffusion processes description and applicability of mathematical methods such as Riemannian geometry and tensor analysis can be useful during development of other semiconductor structures as well. And that is very important and perspective for fabrication of various semiconductor nanostructures.

(1)

The diffusion process in the crystal is considered as having the form of a band with the thickness of H . The diffusion is performed through the window $-l_1 < x^1 < +l_1$, $-l_2 < x^2 < +l_2$ and $x^3 = 0$ by the diffusant being in the gaseous phase with concentration of N_D (see the **Figure 1**). Note that, below the methods of tensor analysis and Riemannian geometry will be applied. That is why we maintain the corresponding formalism with symbols (x^1, x^2, x^3) instead of usual space coordinates (x, y, z) . So as the crystal horizontal sizes are larger than band electrons diffusion length in horizontal directions it is considered to be infinite. In case of H is larger than the diffusion length in the Ox^3 axis direction, the crystal should be considered as infinite as well. Otherwise, i.e., in case of thin crystals, while solving the corresponding boundary problems the influence of bottom $x^3 = -H$ should be taken into account.

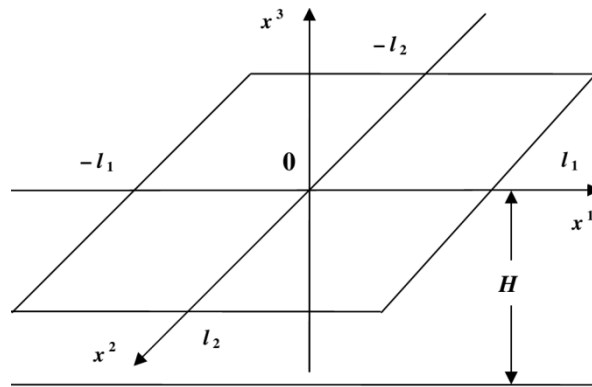


Figure 1. Window for diffusant atoms.

The diffusant atoms penetrate into the crystal through the window points. The rest part of the $x^3 = -H$ surface is covered by the oxide and is impermeable for them. We'll consider here a general case of diffusion process, in particular, take into account that the crystal, $-\infty < x^1 < +\infty$, $-\infty < x^2 < +\infty$ and $-H < x^3 < 0$, in general, is anisotropic and heterogeneous, i.e., diffusion process is characterized by the diffusion tensor,

$$(D^{ik}) = \begin{pmatrix} D^{11} & D^{12} & D^{13} \\ D^{12} & D^{22} & D^{23} \\ D^{13} & D^{23} & D^{33} \end{pmatrix}, \quad (1)$$

providing that all D^{ik} , $i, k = 1, 2, 3$, are the functions of variables (x^1, x^2, x^3) . In these conditions, process is described by the diffusion differential equation:

$$\frac{\partial N}{\partial x} - \frac{\partial}{\partial x^i} \left(D^{ik} \frac{\partial N}{\partial x^k} \right) = 0, \quad t > 0, \quad -\infty < x^1 < +\infty, \quad -\infty < x^2 < +\infty, \quad -H < x^3 < 0, \quad (2)$$

where $N(t, x^1, x^2, x^3)$ is the diffusant atoms concentration. Note that for coinciding upper and lower indices there is realized the summing from 1 to 3:

$$\frac{\partial}{\partial x^i} \left(D^{ik} \frac{\partial N}{\partial x^k} \right) = \frac{\partial}{\partial x^1} \left(D^{11} \frac{\partial N}{\partial x^1} \right) + \frac{\partial}{\partial x^1} \left(D^{12} \frac{\partial N}{\partial x^2} \right) + \dots + \frac{\partial}{\partial x^3} \left(D^{33} \frac{\partial N}{\partial x^3} \right).$$

Here $\| D^{ik} \|$ is the matrix positively determined in all the points. Its components depend not only on the crystal physical properties, but its orientation as well. To simplify the diffusion

investigation we'll mean that crystal is oriented in such a way that $D^{13} = D^{23} = 0$. This condition does not limit the generality of the problem consideration.

Below, instead of parameters D^{ik} , there are introduced the new parameters g^{ik} :

$$D^{ik} = \sqrt{g} g^{ik}, \quad i, k = 1, 2, 3, \quad (3)$$

where g is the determinant of $\|g_{ik}\|$ matrix, the inverse of $\|g^{ik}\|$ matrix:

$$g = \det(g_{ik}) = \begin{vmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{vmatrix}, \quad g^{ip} g_{pk} = \delta_k^i, \quad i, k = 1, 2, 3, \quad (4)$$

$$\delta_k^i = \begin{cases} 1, & i = k \\ 0, & i \neq k \end{cases}, \quad (5)$$

$$\frac{1}{g} = \det(g^{ik}) = \begin{vmatrix} g^{11} & g^{12} & g^{13} \\ g^{12} & g^{22} & g^{23} \\ g^{13} & g^{23} & g^{33} \end{vmatrix}, \quad (6)$$

$$g = D^2, \quad (7)$$

$$D = \det(D^{ik}) = \begin{vmatrix} D^{11} & D^{12} & D^{13} \\ D^{12} & D^{22} & D^{23} \\ D^{13} & D^{23} & D^{33} \end{vmatrix}. \quad (8)$$

That is why according to (3) we have:

$$g^{ik} = \frac{D^{ik}}{D}, \quad i, k = 1, 2, 3. \quad (9)$$

Taking into account these equations, the equation (2) obtains the following form:

$$\frac{\partial N}{\partial t^*} - \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left(\sqrt{g} g^{ik} \frac{\partial N}{\partial x^k} \right) = 0, \quad t^* = \sqrt{g} t > 0, \quad -\infty < x^1 < +\infty, \quad -\infty < x^2 < +\infty, \quad -H < x^3 < 0. \quad (10)$$

In the left part of equation (10), second summand is a covariant divergence [1–4] of the contravariant vector $g^{ik} dN/dx^k$. Thus, equation (10) can be rewritten as follows:

$$\frac{dN}{dt^*} - \left(g^{ik} \frac{dN}{dx^k} \right) = 0, \quad t^* > 0, \quad -\infty < x^1 < +\infty, \quad -\infty < x^2 < +\infty, \quad -H < x^3 < 0. \quad (11)$$

From this differential equation it is apparent that the area occupied by heterogeneous and anisotropic crystal is a curved (for diffusion processes) space with the metric tensor g^{ik} determined by the components D^{ik} according to (9). In this space, the distance between the points $M'(x^{11}, x^{12}, x^{13})$ and $M''(x^{21}, x^{22}, x^{23})$ is the length s of geodesic line arc between them [1], which is determined [1–4] by solution of the following system of usual differential equations with s' for a running length of the geodesic line:

$$\frac{\partial^2 x^k}{\partial s'^2} + \Gamma_{pq}^k \frac{dx^p}{ds'} \frac{dx^q}{ds'} = 0, \quad x^k = \begin{cases} x^{1k}, & s' = 0 \\ x^{2k}, & s' = s \end{cases}, \quad k = 1, 2, 3, \quad (12)$$

$$\Gamma_{ij}^k = \frac{g^{kp}}{2} \left(\frac{\partial g_{ip}}{\partial x^j} + \frac{\partial g_{jp}}{\partial x^i} - \frac{\partial g_{ij}}{\partial x^p} \right), \quad i, j, k = 1, 2, 3 \quad (13)$$

are the Christoffel symbols [1–4]. The first integral of the system (12) has [1] the form:

$$g_{pq} \frac{\partial x^p}{\partial s'} \frac{\partial x^q}{\partial s'} = 1. \quad (14)$$

For practices it is very important to study the diffusion process in homogeneous, but anisotropic crystal. The metric tensor g^{ik} components are the constants as the D^{ik} tensor components are constants by their definition. But for constant g^{ik} , according to the equation (13), the Christoffel symbols are zero, $\Gamma_{ij}^k = 0$, and the system (12) takes the form:

$$\frac{d^2 x^k}{ds'^2} = 0, \quad x^k = \begin{cases} x'^k, & s' = 0 \\ x''^k, & s' = s \end{cases}. \quad (15)$$

Solutions of the last system are:

$$x^k = x'^k + \frac{s'}{s}(x''^k - x'^k), \quad (16)$$

$$s^2 = g_{pq}(x''^p - x'^p)(x''^q - x'^q). \quad (17)$$

To investigate the diffusion process we'll apply below the Green's function method, for which it is necessary to introduce notion of fundamental solution of the differential equation (11), being the diffusants concentration from a point source in infinite 3D space [2, 3]:

$$N(t^*, x^1, x^2, x^3; t'^*, x'^1, x'^2, x'^3) = \frac{1}{8(\pi(t^* - t'^*))^{3/2}} \exp\left(-\frac{s^2(x^1, x^1, x^1; x'^1, x'^2, x'^3)}{4(t^* - t'^*)}\right), \quad (18)$$

where x^k and x'^k are the coordinates of two points in area under the consideration, s is the length of geodesic line between them and t and t' are two moments of time at $t' \leq t$.

In the general case of heterogeneous crystal, for determination the functional dependence analogous to (17) it should be solved the system (12) with corresponding boundary conditions in regard to unknown functions $x^k = x^k(s)$ and applied the equation (14) [2, 3].

Let's note an important property of the fundamental equation (18) that at $t'^* \neq t^*$ or $t' \neq t$ it is a regular function in the whole 3D space and tends to zero in infinity $s \rightarrow \infty$. At $t'^* \rightarrow t^*$ this function tends to zero in almost all the points of infinite 3D space excluding $M(x^1, x^2, x^3)$ point. At this point, i.e., when $x'^k = x^k$, it tends to infinity as $\sim 1/(t^* - t'^*)^{3/2}$. And in all the other points of whole infinite 3D space, it tends to 1. Thus, when $t'^* \rightarrow t^*$, the limiting function possesses properties of the Dirac $\delta(s)$ function [2, 3]. These properties of fundamental solution (18) will be applied below while constructing Green's function.

(2)

In the isoplanar technology, two different diffusion processes, A and B, can take place.

Process A means that for diffusant atoms the window is not covered by oxide. In gaseous phase, they penetrate into the crystal through this window and scatter in the crystal depth. In the window points, the diffusant atoms' concentration is equal to their concentration $N_D(t, x^1, x^2)$ in gaseous phase. Control of functional dependence of N_D on variables x^1 and x^2 in the window area in case under the consideration is an unrealizable procedure. However, we have studied the boundary problem assuming that such dependence is known. Consequently, the obtained results can be applied in other tasks with known $N_D(t, x^1, x^2)$ functions.

Thus, in window points the below equation should be valid:

$$N(t, x^1, x^2, x^3) = N_D(t, x^1, x^2), \quad t > 0, \quad -l_1 < x^1 < +l_1, \quad -l_2 < x^2 < +l_2, \quad x^3 = 0, \quad (19)$$

where $N_D(t, x^1, x^2)$ is a known function of its arguments.

Rest (out of the window) part of the surface, $x^3 = 0$, is covered by the oxide and that is why the diffusant atoms are not penetrable. At the surface $x^3 = 0$, the condition

$$\frac{\partial N}{\partial \nu} = g^{pq} \nu_p \frac{\partial N}{\partial x^q} = 0, \quad -l_1 < x^1 < +l_1, \quad -l_2 < x^2 < +l_2, \quad x^3 = 0, \quad (20)$$

is valid. Here $\vec{\nu}$ is the unit vector normal to $x^3 = 0$ surface. In case under the consideration, its components are $\vec{\nu}(0,0,1/\sqrt{g^{33}})$. That is why the equation (20) takes the form:

$$g^{3q} \frac{\partial N}{\partial x^q} = 0, \quad -l_1 < x^1 < +l_1, \quad -l_2 < x^2 < +l_2, \quad x^3 = 0, \quad (21)$$

If the crystal is oriented in such a way that $g^{13} = g^{23} = 0$, then we finally have:

$$\frac{\partial N}{\partial x^3} = 0, \quad -l_1 < x^1 < +l_1, \quad -l_2 < x^2 < +l_2, \quad x^3 = 0, \quad (22)$$

Below we'll exploit this very convenient condition.

Process B means that the window is covered by oxide. This case can take place in the process of oxidation, which is carried out at high temperatures. Simultaneously, there occurs a redistribution of diffusant atoms in the crystal depth, which have been introduced at the previous stage of diffusion. When all the $x^3 = 0$ surface is oxidized, the diffusion equation is:

$$\frac{\partial N}{\partial x^3} = 0, \quad t > 0, \quad -\infty < x^1 < +\infty, \quad -\infty < x^2 < +\infty, \quad x^3 = 0. \quad (23)$$

For thin crystals, analogous condition is valid on its bottom $x^3 = -H$:

$$\frac{\partial N}{\partial x^3} = 0, \quad t > 0, \quad -\infty < x^1 < +\infty, \quad -\infty < x^2 < +\infty, \quad x^3 = -H. \quad (24)$$

If in the initial moment of diffusion, $t = 0$, the crystal was free of diffusant atoms then it is valid the initial condition:

$$N(t, x^1, x^2, x^3) = 0, \quad t > 0, \quad -\infty < x^1 < +\infty, \quad -\infty < x^2 < +\infty, \quad -H < x^3 < 0. \quad (25)$$

Otherwise

$$N(t, x^1, x^2, x^3) = N_0(x^1, x^2, x^3), \quad t > 0, \quad -\infty < x^1 < +\infty, \quad -\infty < x^2 < +\infty, \quad -H < x^3 < 0, \quad (26)$$

where $N_0(x^1, x^2, x^3)$ is the known function determined by the previous diffusion processes.

(3)

Using the boundary and initial conditions given here, it is possible to analyze various boundary problems describing above mentioned diffusion processes.

For process A in a thin crystal, to find a regular solution of the differential equation (11) satisfying the boundary conditions (19) and (22) and the initial condition (26), and in the infinity tending to zero, equation should be added with boundary condition (24) as well. Note that under the regular function we mean such a function, which is continuous and has continuous first order partial derivatives and limited second order partial derivatives.

For process B in a thin crystal, to find a regular solution of differential equation (11) in partial derivatives satisfying the boundary condition (23) and the initial condition (21), and in the infinity tending to zero, again the boundary condition (24) should be introduced.

Solution of these boundary problems are the sole. When $N_0(x^1, x^2, x^3) = 0$ in the crystal bulk and $H_D(t, x^1, x^2) = 0$ in the windows area, these problems have only trivial solution: $N(t, x^1, x^2, x^3) = 0$. To obtain non-trivial solutions, let's multiply the equation (11) on

$N(t, x^1, x^2, x^3)$ and integrate gotten equation by t^* from 0 to t^* , and by x^1 , x^2 and x^3 on the crystal volume: $\frac{1}{2} \int_{-\infty}^{+\infty} dx^1 \int_{-\infty}^{+\infty} dx^2 \int_{-H}^0 dx^3 \sqrt{g} N^2 + \int_0^{t^*} dt^* \int_{-\infty}^{+\infty} dx^1 \int_{-\infty}^{+\infty} dx^2 \int_{-H}^0 dx^3 \sqrt{g} g^{ik} \frac{\partial N}{\partial x^i} \frac{\partial N}{\partial x^k} = 0$. In deriving of this equation, there were included studied boundary and initial conditions. As $\|g^{ik}\|$ is a positively determined matrix, $\int_{-\infty}^{+\infty} dx^1 \int_{-\infty}^{+\infty} dx^2 \int_{-H}^0 dx^3 \sqrt{g} N^2 = 0$, and then $N(t, x^1, x^2, x^3) \equiv 0$, $t > 0$, $-\infty < x^1 < +\infty$, $-\infty < x^2 < +\infty$, $-H < x^3 < 0$, i.e., the solutions are sole.

To solve A and B boundary problems, there will be applied the Green's function method. Taking into account that Green's function itself is a solution of certain boundary problem, let's assume the function $K(t^*, x^1, x^2, x^3; t'^*, x'^1, x'^2, x'^3)$ of 8 independent variables with specified values of 4 of them, t^* , x^1 , x^2 and x^3 , satisfy the following equations:

$$\begin{aligned}
 \frac{\partial K}{\partial t'^*} + \left(g^{ik} \frac{\partial K}{\partial x'^k} \right) &= 0, \quad t'^* > 0, \quad -\infty < x'^1 < +\infty, \quad -\infty < x'^2 < +\infty, \quad -H < x'^3 < 0, \\
 K &= 0, \quad t'^* > 0, \quad -l_1 < x'^1 < +l_1, \quad -l_2 < x'^2 < +l_2, \quad x'^3 = 0, \\
 \frac{\partial K}{\partial x'^3} &= 0, \quad t'^* > 0, \quad -l_1 < x'^1 < +l_1, \quad -l_2 < x'^2 < +l_2, \quad x'^3 = 0.
 \end{aligned} \quad (27)$$

Besides, $K \rightarrow \delta(s)$ at $t'^* \rightarrow t^*$, when $t'^* > 0$, $-\infty < x'^1 < +\infty$, $-\infty < x'^2 < +\infty$ and $-H < x'^3 < 0$, and $K \rightarrow 0$ at $s \rightarrow \infty$, where s is the geodesic line arc length between the points $M(x^1, x^2, x^3)$ and $M'(x'^1, x'^2, x'^3)$. For thin crystal, the system (27) should be added with the condition:

$$\frac{\partial K}{\partial x'^3} = 0, \quad t'^* > 0, \quad -l_1 < x'^1 < +l_1, \quad -l_2 < x'^2 < +l_2, \quad x'^3 = -H. \quad (28)$$

The function satisfying these conditions is called the Green's function of boundary problem A.

Let the function K of 8 independent variables at fixed values of 4 variables, t^* , x^1 , x^2 and x^3 , meets the following conditions:

$$\begin{aligned}
 \frac{\partial K}{\partial t'^*} + g^{ik} \frac{\partial K}{\partial x'^k} &= 0, \quad t'^* > 0, \quad -\infty < x'^1 < +\infty, \quad -\infty < x'^2 < +\infty, \quad -H < x'^3 < 0, \\
 \frac{\partial K}{\partial x'^3} &= 0, \quad t'^* > 0, \quad -\infty < x'^1 < +\infty, \quad -\infty < x'^2 < +\infty, \quad x'^3 = 0.
 \end{aligned} \quad (29)$$

Besides, $K \rightarrow \delta(s)$ at $t'^* \rightarrow t^*$, when $t'^* > 0$, $-\infty < x'^1 < +\infty$, $-\infty < x'^2 < +\infty$ and $-H < x'^3 < 0$, $K \rightarrow 0$ at $s \rightarrow \infty$, and in regard to variables t^* , x^1 , x^2 and x^3 this function meets the differential equation (11). For thin crystal, these conditions again should be added with (28). Function satisfying these conditions is called the Green's function of boundary problem B.

The boundary problem (27) is very complex and it is practically impossible to find its solution. But, solution of the boundary problem (29) is determined [2, 3] by simple expression:

$$K(t^*, x^1, x^2, x^3; t'^*, x'^1, x'^2, x'^3) = \frac{1}{2\sqrt{\pi(t^* - t'^*)^3}} \left(\exp\left(-\frac{s^2(x^1, x^2, x^3; x'^1, x'^2, x'^3)}{4(t^* - t'^*)}\right) + \exp\left(-\frac{s^2(x^1, x^2, x^3; x'^1, x'^2, -x'^3)}{4(t^* - t'^*)}\right) \right). \quad (30)$$

This function for variables t'^* , x'^1 , x'^2 and x'^3 satisfies the equation of boundary problem (23) so as contains the variable t'^* with negative sign and the variable t^* with positive sign. That is why for variables t^* , x^1 , x^2 and x^3 it satisfies the differential equation (11). The boundary condition of the system (29), when $x'^3 = 0$, is satisfied automatically as the first term in the right part of the equation (30) contains the variable x'^3 with positive sign and the second

– with the negative sign. The validity of the system penultimate condition (29) results from the structure of the first term – it is identical to expression (18); and fact that the second term is a regular function (nowhere in the band $s(x^1, x^2, x^3; x^{11}, x^{12}, x^{13}) \neq 0$ has the peculiarities) in the infinite band $-\infty < x^{11} < +\infty$, $-\infty < x^{12} < +\infty$ and $-H < x^{13} < 0$. More details possible see in [2, 3].

Below, the expression (30) will be applied not only for solution of boundary problem B, but boundary problem A as well. Of course, it will appear the additional difficulties, which will be overcome through the corresponding ways. In this connection, the Green's function of boundary problem B determined by the equation (30) we'll call as modified Green's function of boundary problem A.

Diffusion in homogeneous but anisotropic crystal is of great interest for microelectronics, in particular, while fabrication thin film structures. As metric tensor (g^{ik}) contains the constant components, s is determined by simple expression (17) and the Green's function of boundary problem B, i.e., the modified Green's function of boundary problem A, equals:

$$K(t, x^1, x^2, x^3; t', x^{11}, x^{12}, x^{13}) = \frac{1}{2\sqrt{\pi\sqrt{g}(t-t')^3}} \left(\exp\left(-\frac{\rho^2 + g_{33}(x^3 - x^{13})^2}{4\sqrt{g}(t-t')}\right) + \exp\left(-\frac{\rho^2 + g_{33}(x^3 + x^{13})^2}{4\sqrt{g}(t-t')}\right) \right), \quad (31)$$

$$\rho^2 = g_{\alpha\beta}(x - x'^\alpha)(x - \beta x'). \quad (32)$$

In the right part, summation indices are: $\alpha, \beta = 1, 2$.

In case of thin heterogeneous and anisotropic crystal

$$K(t^*, x^1, x^2, x^3; t'^*, x^{11}, x^{12}, x^{13}) = \frac{1}{2\sqrt{\pi(t^* - t'^*)^3}} \sum_{k=-\infty}^{k=+\infty} \left(\exp\left(-\frac{s^2(x^1, x^2, x^3; x^{11}, x^{12}, 2(k+1)H + x^{13})}{4(t^* - t'^*)}\right) + \exp\left(-\frac{s^2(x^1, x^2, x^3; x^{11}, x^{12}, -2kH - x^{13})}{4(t^* - t'^*)}\right) \right). \quad (33)$$

Similarly, for homogeneous and anisotropic crystal, which fills up a thin layer, we have

$$K(t, x^1, x^2, x^3; t', x^{11}, x^{12}, x^{13}) = \frac{1}{2\sqrt{\pi\sqrt{g}(t-t')^3}} \sum_{k=-\infty}^{k=+\infty} \left(\exp\left(-\frac{\rho^2 + g_{33}(x^3 - 2(k+1)H - x^{13})^2}{4\sqrt{g}(t-t')}\right) + \exp\left(-\frac{\rho^2 + g_{33}(x^3 + 2kH + x^{13})^2}{4\sqrt{g}(t-t')}\right) \right). \quad (34)$$

(4)

As is above mentioned, it is practically difficult to realize the solution of boundary problem (27) in detail because it is difficult to determine the Green's function of boundary problem A. However, the Green's function of boundary problem B is quite simple and is determined by equations (31), (33) or (34) depending on practical situations. We'll apply this Green's function for solving the boundary problem A as well.

Rewrite the equation (11) into variables t^* , x^{11} , x^{12} and x^{13} multiplying it by Green's function K and adding to the first equation of system (29) multiplied by N :

$$\frac{\partial(KN)}{\partial t'^*} + g^{ik} \left(N \frac{\partial K}{\partial x^{ik}} - K \frac{\partial N}{\partial x^{ik}} \right) = 0. \quad (35)$$

Let's multiply this equation by $dx^{11} dx^{12} dx^{13} \sqrt{g}$, the volume element invariant form [1–4], and dt^* and integrate within the limits: $0 < t'^* < t^*$, $-\infty < x^{11} < +\infty$, $-\infty < x^{12} < +\infty$ and $-H < x^{13} < 0$. For Green's function K rather fast tending to 0 at $s \rightarrow \infty$, we receive:

$$\int_{-\infty}^{+\infty} dx^{11} \int_{-\infty}^{+\infty} dx^{12} \int_{-H}^0 dx^{13} \sqrt{g} KN \Big|_{t'^*=t} - \int_{-\infty}^{+\infty} dx^{11} \int_{-\infty}^{+\infty} dx^{12} \int_{-H}^0 dx^{13} \sqrt{g} KN \Big|_{t'^*=0} =$$

$$= \int_0^{t^*} dt'^* \int_{-\infty}^{+\infty} dx^{11} \int_{-\infty}^{+\infty} dx^{12} \sqrt{g} g^{33} \left(K \frac{\partial N}{\partial x^{13}} - N \frac{\partial K}{\partial x^{13}} \right) \Big|_{x^{13}=0} + \int_0^{t^*} dt'^* \int_{-\infty}^{+\infty} dx^{11} \int_{-\infty}^{+\infty} dx^{12} \sqrt{-g} g^{33} \left(K \frac{\partial N}{\partial x^{13}} - N \frac{\partial K}{\partial x^{13}} \right) \Big|_{x^{13}=-H}. \quad (36)$$

Second term in the right part of the obtained equality takes into account the crystal influence at the depth $x^3 = -H$. However, according to the boundary conditions for functions K and N , $\partial K / \partial x^3 = 0$ and $\partial N / \partial x^3 = 0$ at $x^3 = -H$, this term identically equals to zero. According to the penultimate condition of system (29), the first term in the left part of the last equality is equal to $N(t, x^1, x^2, x^3)$. From the initial condition of boundary problems A and B, $N = N_0(x^1, x^2, x^3)$ at $t = 0$, (36) is finally converted into the equality:

$$N(x^1, x^2, x^3) = \int_{-\infty}^{+\infty} dx^1 \int_{-\infty}^{+\infty} dx^2 \int_{-H}^0 dx^3 \sqrt{g} N_0(x^1, x^2, x^3) K(t^*, x^1, x^2, x^3; 0, x^1, x^2, x^3)^3 + \int_0^{t^*} dt^* \int_{-\infty}^{+\infty} dx^1 \int_{-\infty}^{+\infty} dx^2 \sqrt{g} g^{33} \left(K \frac{\partial N}{\partial x^3} - N \frac{\partial K}{\partial x^3} \right) \Big|_{x^3=0}. \quad (37)$$

In its derivation, the conditions $g^{13} = g^{23} = 0$ have been taken into account. In case of thick crystal in the first term of this equality the integration on variable x^3 should be realized within the limits from $-\infty$ to 0 .

Let's start with boundary problem A. As it has been noted above, we shall apply function K determined by the equality (30). It satisfies the condition $\partial K / \partial x^3 = 0$ on the whole plane $x^3 = 0$. That is why in the second term in the right part of the equality (37) the subintegral function is connected to $g^{33} K \partial N / \partial x^3 \Big|_{x^3=0}$ and then $\partial N / \partial x^3 = 0$ out of window: $-l_1 < x^1 < +l_1$, $-l_2 < x^2 < +l_2$ and $x^3 = 0$. Finally, (37) acquires such an appearance:

$$N(t, x^1, x^2, x^3) = \frac{1}{2} \int_{-\infty}^{+\infty} dx^1 \int_{-\infty}^{+\infty} dx^2 \int_{-\infty}^0 dx^3 \frac{N_0(x^1, x^2, x^3)}{\sqrt{\pi \sqrt{g} t^3}} \left(\exp \left(-\frac{s^2(x^1, x^2, x^3; x^1, x^2, x^3)}{4\sqrt{g} t} \right) + \exp \left(-\frac{s^2(x^1, x^2, x^3; x^1, x^2, -x^3)}{4\sqrt{g} t} \right) \right) + \frac{1}{2} \int_0^{\sqrt{g} t} dt^* \int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{g}{\pi(\sqrt{g} t - t^*)^3}} g^{33} \exp \left[-\frac{s^2(x^1, x^2, x^3; x^1, x^2, 0)}{4(\sqrt{g} t - t^*)} \right] \zeta(t^*, x^1, x^2), \quad (38)$$

where

$$\zeta(t^*, x^1, x^2) = \frac{\partial N}{\partial x^3} \Big|_{x^3=0} \quad (39)$$

is an unknown function, expression of which is related with applied modified Green's function.

The first term in the right part of the obtained equality is completely determined by the function satisfying the differential equation (11) and the initial condition of boundary problem A at $t = 0$: when $t \rightarrow 0$ the K function coincides with Dirac $\delta(s)$ function.

In case of making the thin film structure with $N_0(x^1, x^2, x^3) \equiv 0$ inside crystal, the taking into account the relation $s^2 = \rho^2 + g_{33}(x^3)^2$ (see (31) and (32)) converts (37) into form

$$N(t, x^1, x^2, x^3) = \int_0^{\sqrt{g} t} dt^* \int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{g}{\pi(\sqrt{g} t - t^*)^3}} g^{33} \exp \left(-\frac{\rho^2 + g_{33}(x^3)^2}{4(\sqrt{g} t - t^*)} \right) \zeta(t^*, x^1, x^2). \quad (40)$$

Let's determine the unknown function $\zeta(t^*, x^1, x^2)$ within ranges: $0 < t^* < \sqrt{g} t$, $-l_1 < x^1 < +l_1$ and $-l_2 < x^2 < +l_2$ by means of condition (19) of boundary problem A from (40):

$$\int_0^{\sqrt{g} t} dt^* \int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{g}{\pi(\sqrt{g} t - t^*)^3}} g^{33} \exp \left(-\frac{\rho^2}{4(\sqrt{g} t - t^*)} \right) \zeta(t^*, x^1, x^2) = N_D(t, x^1, x^2). \quad (41)$$

This equality is a Volterra- and Fredholm-type integral equations relative to variable t and variables x^1 and x^2 , respectively. Its solution determines the sought function $\zeta(t^*, x^1, x^2)$ in the points of window. After inserting this function in the right part of the equation (40), we'll obtain the general expression for calculating the diffusant concentration $N(t, x^1, x^2, x^3)$ in any point of the crystal for any moment of time.

In case of thin crystal, instead of Green's function (30) it should be applied a function determined by the equality (34). The whole remained procedure is similar to that of previous.

For the boundary problem B on the plane $x^3 = 0$ the following condition is valid: $\partial K / \partial x^3 = 0$, $\partial N / \partial x^3 = 0$, $-\infty < x^1 < +\infty$, $-\infty < x^2 < +\infty$ and $x^3 = 0$. That is why the second term in the right part of the equality (37) is zero and then solution of the boundary problem B obtains such a form:

$$N(t, x^1, x^2, x^3) = \frac{1}{2} \int_{-\infty}^{+\infty} dx^1 \int_{-\infty}^{+\infty} dx^2 \int_{-\infty}^0 dx^3 \sqrt{\frac{g}{\pi t^3}} N_0(x^1, x^2, x^3) \left(\exp\left(-\frac{\rho^2 + g_{33}(x^3 - x'^3)^2}{4\sqrt{g}t}\right) + \exp\left(-\frac{\rho^2 + g_{33}(x^3 + x'^3)^2}{4\sqrt{g}t}\right) \right). \quad (42)$$

This equality can be used for calculation of redistribution of diffusant atoms in the crystal volume during realization of other high-temperature thermal processes in a technological cycle of preparation of isoplanar structures, e.g., while the oxidation.

(5)

In the case of homogeneous but anisotropic crystal, the components of metric tensor g^{ik} are constants, like the diffusion coefficients D^{ik} . Then

$$\int_0^t dt' \int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{\sqrt{g}}{\pi(t-t')^3}} g^{33} \exp\left(-\frac{g_{\alpha\beta}(x^\alpha - x'^\alpha)(x^\beta - x'^\beta)}{4\sqrt{g}(t-t')}\right) \zeta(t', t^1, t^2) = N_D. \quad (43)$$

Below we assume that $N_D = \text{const}$ so as practically it is not possible to control the concentration of a diffusant in various points of the window depending on the coordinates of points of window and time.

Let's assume that in some interval of time $0 < t < t_0$, solution of this integral equation is known, i.e., $\zeta(t, x^1, x^2)$ is considered as a known function at $0 < t < t_0$, $-l_1 < x^1 < +l_1$ and $-l_2 < x^2 < +l_2$. Then in the interval of time $0 < t < t_0 + \Delta t$, where Δt is some small (in comparison with total time of diffusion) quantity, from (43) we obtain:

$$\int_{t_0}^{t_0+\Delta t} dt' \int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{\sqrt{g}}{\pi(t_0+\Delta t-t')^3}} g^{33} \exp\left(-\frac{g_{\alpha\beta}(x^\alpha - x'^\alpha)(x^\beta - x'^\beta)}{4\sqrt{g}(t_0+\Delta t-t')}\right) \zeta(t_0, x^1, x^2) = f_0(t, x^1, x^2), \quad (44)$$

where

$$f_0(t_0, x^1, x^2) = N_D - \int_0^{t_0} dt' \int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{\sqrt{g}}{\pi(t_0+\Delta t-t')^3}} g^{33} \exp\left(-\frac{g_{\alpha\beta}(x^\alpha - x'^\alpha)(x^\beta - x'^\beta)}{4\sqrt{g}(t_0+\Delta t-t')}\right) \zeta(t', x^1, x^2) \quad (45)$$

is the known function. Taking into account that Δt is small, the integration by t' in the equation (44) is possible to alter by approximated value and instead (44) we'll obtain:

$$\int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{\sqrt{g}}{\pi\Delta t}} g^{33} \exp\left(-\frac{g_{\alpha\beta}(x^\alpha - x'^\alpha)(x^\beta - x'^\beta)}{4\sqrt{g}\Delta t}\right) \zeta(t_0, x^1, x^2) \approx f(t_0, x^1, x^2, x^3). \quad (46)$$

At $t_0 = 0$, according to (45), $f(0, x^1, x^2) = N_D$ and from (46) we obtain:

$$\int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{\sqrt{g}}{\pi\Delta t}} g^{33} \exp\left(-\frac{g_{\alpha\beta}(x^\alpha - x'^\alpha)(x^\beta - x'^\beta)}{4\sqrt{g}\Delta t}\right) \zeta(0, x^1, x^2) \approx N_D. \quad (47)$$

Applying the known methods of integrating, this integral equation comes to linear system of algebraic equations, solution of which is the sought function $\zeta(0, x^\mu, x^\nu)$ in some points x^μ and x^ν of the window:

$$\mu = 1, 2, 3, \dots, m, \quad \nu = 1, 2, 3, \dots, n. \quad (48)$$

Now let's assume that $t_0 = \Delta t$, then from (46) we'll receive:

$$\int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx^2 \sqrt{\frac{g}{\pi \Delta t}} g^{33} \exp\left(-\frac{g_{\alpha\beta}(x^\alpha - x'^\alpha)(x^\beta - x'^\beta)}{4\sqrt{g}\Delta t}\right) \zeta(\Delta t, x^1, x^2) \approx f(\Delta t, x^1, x^2, x^3), \quad (49)$$

where

$$f_0(\Delta t, x^1, x^2) \approx N_D - \int_0^{\Delta t} dt' \int_{-l_1}^{+l_1} dx^1 \int_{-l_2}^{+l_2} dx'^2 \sqrt{\frac{g}{\pi(2\Delta t - t')^3}} g^{33} \exp\left(-\frac{g_{\alpha\beta}(x^\alpha - x'^\alpha)(x^\beta - x'^\beta)}{4\sqrt{g}(2\Delta t - t')}\right) \zeta(t', x^1, x'^2). \quad (50)$$

This unknown function $\zeta(0, x^1, x^2)$ is determined by solution of preceding integral equation. Note that the integral equations (48) and (49) differ from each other only by their right parts. So, similarly to previous solution of integral equation (40) the sought function $\zeta(\Delta t, x^\mu, x^\nu)$ can be determined in the window points in the Δt moment of time.

Continuation of this process will determine the value of sought function $\zeta(t, x^1, x^2)$ at time moments $t = 0, \Delta t, 2\Delta t, \dots$ in discrete points of $M_{\mu\nu}(x^\mu, x^\nu)$ of a window. The diffusant atoms concentration in any desirable point of a crystal in any moment of time is determined according to (40) after substitution function $\zeta(t, x^1, x^2)$ values in its right part.

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