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Solutions modeling of nonlinear equation of diffusion for three dimensions case

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Abstract. We have made a practical consideration of an important case of nonlinear diffusion of impurities in a three-dimensional case through square window in the x, y plane for the production of electronic devices and evaluation of its parameters. The nonlinear diffusion coefficients for diffusion in x, y, z directions are proportional to the concentration of impurities. The three-dimensional nonlinear diffusion equation was transformed using similarity variables. The approximate analytical solution of the transformed equation expressed by Taylor series approximate expansion for three similarity variables about the maximum impurities penetration points in x, y, z axes including the square terms.

Keywords: nonlinear diffusion equation, approximate analytical solution, similarity variables.

Introduction

The classical linear diffusion equation is derived from the Fokker–Planck equation which was obtained by assuming, that the process is slow. We see that fitting an experimental profile tail region of impurities to the classical solution $erfc(x/2\sqrt{(Dt)})$ tail region, where linear diffusion must occur with large velocity, is physically non acceptable and cannot be fitted with experiment [7, 14]. Any diffusion theory and equation must conform to Brownian motion from where follows that the diffusion velocity and maximum penetration depth of impurity atoms must be finite [3, 8, 10]. The diffusion coefficient must be equal to zero in the region where the impurities are absent. According to this realistic assumption the following nonlinear diffusion equation was proposed [7]

$$\frac{\partial N}{\partial t} = \frac{\partial}{\partial x}\left(D(N)\frac{\partial N}{\partial x}\right) \tag{1}$$

with the flux j, when the nonlinear diffusion coefficient $D(N)$ was directly proportional to the impurities concentration N [7, 3, 14]

$$j = -D(N)\frac{\partial N}{\partial x}, \qquad D(N) = \frac{N}{N_s}D = \frac{N}{N_s}D_0 e^{-\frac{E}{kT}}, \tag{2}$$

where D is diffusion coefficient for linear diffusion equation, N_s is impurities concentration at the source [7, 3]. D is defined by the pre-exponential factor D_0, Boltzmanns constant k, temperature T, the activation energy E. From the above presented Eq. (1) and [8, 10] we can obtain the nonlinear diffusion equation in the three-dimensional case

$$\frac{\partial N}{\partial t} = \frac{\partial}{\partial x}\left(D(N)\frac{\partial N}{\partial x}\right) + \frac{\partial}{\partial y}\left(D(N)\frac{\partial N}{\partial y}\right) + \frac{\partial}{\partial z}\left(D(N)\frac{\partial N}{\partial z}\right), \tag{3}$$

$$D(N) = \frac{1}{N_s} DN(x,y,z) \tag{4}$$

with linear diffusion coefficient (2) D according to the x, y and z axes when off-diagonal elements equal zero [2]. In this case jumps of diffusing particles can occur in the x, y and z axis in orthogonal directions. It can happen in crystals with cubic lattice [2].

1 The approximate solution of the three-dimensional nonlinear diffusion equation

The nonlinear diffusion equation (3) will be solved introducing similarity variables [10]

$$\begin{gathered} \xi_1 = \frac{|x| - h}{\sqrt{(Dt)}}, \qquad \xi_2 = \frac{|y| - h}{\sqrt{(Dt)}}, \qquad \xi_3 = \frac{z}{\sqrt{(Dt)}}, \quad h \leqslant |x|,\ h \leqslant |y|, \\ 0 \leqslant z \leqslant z_0, \qquad z_0 = \xi_{30}\sqrt{(Dt)}, \\ 0 \leqslant \xi_1 \leqslant \xi_{10}, \qquad 0 \leqslant \xi_2 \leqslant \xi_{20}, \qquad 0 \leqslant \xi_3 \leqslant \xi_{30} \end{gathered} \tag{5}$$

describing the square source with the diagonals length $2h$ and defining the corners in the x, y plane. The size $2h$ depends on planar technologies and can be $1\ \mu\text{m} \leqslant 2h \leqslant 1$ cm. For solution of (3)

$$N(x,y,z,t) = N_s f(\xi_{1d}, \xi_{2d}, \xi_{3d}), \tag{6}$$

$$\sum_{i=1}^{3}\left(2\frac{\partial}{\partial \xi_{id}}\left(f\frac{\partial f}{\partial \xi_{id}}\right) + \xi_{id}\frac{\partial f}{\partial \xi_{id}} + \xi_{i0}\frac{\partial f}{\partial \xi_{id}}\right) = 0 \tag{7}$$

expressed in new variables

$$\begin{gathered} \xi_{1d} = \xi_1 - \xi_{10}, \qquad \xi_{2d} = \xi_2 - \xi_{20}, \qquad \xi_{3d} = \xi_3 - \xi_{30}, \\ -\xi_{10} \leqslant \xi_{1d} \leqslant 0, \qquad -\xi_{20} \leqslant \xi_{2d} \leqslant 0, \qquad -\xi_{30} \leqslant \xi_{3d} \leqslant 0, \end{gathered} \tag{8}$$

we will use the approximate Taylor power expansion [11, 6] about maximum penetration points ξ_{10}, ξ_{20}, ξ_{30} of impurities. The approximate solution $f(\xi_1, \xi_2, \xi_3)$ of (7) can be presented by the Taylor series of three variables expanded [11]

$$\begin{aligned} f(\xi_1,\xi_2,\xi_3) = {} & f(P_0) + \sum_{i=1}^{3}(\xi_i - \xi_{i0})\frac{\partial f}{\partial \xi_i}\bigg|_{P_0} \\ & + \frac{1}{2!}\sum_{i=1}^{3}\sum_{j=1}^{3}(\xi_i - \xi_{i0})(\xi_j - \xi_{j0})\frac{\partial^2}{\partial \xi_i \xi_j}\bigg|_{P_0} + R_3 \end{aligned} \tag{9}$$

at the same point $P_0 = P_0(\xi_{10}, \xi_{20}, \xi_{30})$ where we included boundary condition $f(P_0) = 0$ and dropped the terms R_3 of order 3 and higher. In this case we have

$$f(\xi_1, \xi_2, \xi_3) = \sum_{i=1}^{3} a_i(\xi_i - \xi_{i0}) + a_{3+i}(\xi_i - \xi_{i0})^2 + a_7(\xi_1 - \xi_{10})(\xi_2 - \xi_{20}) + (a_8(\xi_1 - \xi_{10}) + a_9(\xi_2 - \xi_{20}))(\xi_3 - \xi_{30}) \qquad (10)$$

When the window for impurities introduction has the square form we must take in the presented approximate solution requirement of symmetry

$$\xi_{10} = \xi_{20}, \qquad a_2 = a_1, \qquad a_5 = a_4, \qquad a_9 = a_8. \qquad (11)$$

Substituting (10) into (7) and equating collected coefficients at ξ_{id}^n with $n = 0, 1$, $i = 1, 2, 3$ to zero and using boundary conditions

$$f(-\xi_{10}, -\xi_{20}, -\xi_{30}) = 1, \qquad \xi_1 = 0, \qquad \xi_2 = 0, \qquad \xi_3 = 0, \qquad (12)$$

$$f(0, -\xi_{20}, -\xi_{30}) = 0, \qquad \xi_1 = \xi_{10}, \qquad \xi_2 = 0, \qquad \xi_3 = 0, \qquad (13)$$

$$f(-\xi_{10}, 0, -\xi_{30}) = 0, \qquad \xi_1 = 0, \qquad \xi_2 = \xi_{20}, \qquad \xi_3 = 0, \qquad (14)$$

$$f(-\xi_{10}, -\xi_{20}, 0) = 0, \qquad \xi_1 = 0, \qquad \xi_2 = 0, \qquad \xi_3 = \xi_{20} \qquad (15)$$

defining relative concentration of impurities in the center of the square (12) and in the maximum penetration depths ξ_{10}, ξ_{20}, ξ_{30} according to coordinate axes x, y, z (13), (14), (15) consequently.

Then we obtained the following system of equations:

$$4a_1^2 + 2a_3^2 + a_1\xi_{10} + a_1\xi_{20} + a_3\xi_{30} = 0, \qquad (16)$$

$$a_1 + 16a_1a_4 + 4a_1a_7 + 4a_3a_8 + 4a_1a_6 + 2a_4\xi_{10} + a_8\xi_{30} + a_7\xi_{20} = 0, \qquad (17)$$

$$a_3 + 8a_1a_8 + 8a_3a_4 + 12a_3a_6 + a_8\xi_{10} + a_8\xi_{20} + 2a_6\xi_{30} = 0, \qquad (18)$$

$$4a_1a_7 + 16a_1a_4 + 4a_1a_6 + 4a_3a_8 + 2a_4\xi_{20} + a_7\xi_{10} + a_8\xi_{30} + a_1 = 0, \qquad (19)$$

$$-a_1\xi_{10} - a_1\xi_{20} - a_3\xi_{30} + a_4\xi_{10}^2 + a_4\xi_{20}^2 + a_6\xi_{30}^2 + a_7\xi_{10}\xi_{20} + a_8\xi_{10}\xi_{30} + a_8\xi_{20}\xi_{30} = 1, \qquad (20)$$

$$-a_1\xi_{20} - a_3\xi_{30} + a_4\xi_{10}^2 + a_6\xi_{30}^2 + a_8\xi_{20}\xi_{30} = 0, \qquad (21)$$

$$-a_1\xi_{10} - a_3\xi_{30} + a_4\xi_{10}^2 + a_6\xi_{30}^2 + a_8\xi_{10}\xi_{30} = 0, \qquad (22)$$

$$-a_1\xi_{10} - a_1\xi_{20} + a_4\xi_{10}^2 + a_4\xi_{20}^2 + a_7\xi_{10}\xi_{20} = 0 \qquad (23)$$

Last equation we obtained requiring that Eq. (10) must also be satisfied [5] for one dimension case [10] and satisfy boundary condition at ξ_{30}.

The algebraic expressions are quite complex. The formation and solution of a system of equations is made by using the computer algebra system Maple 14. We supposed that the impurities are spreading in z direction approximately like in a one dimension case [6] and then we can substitute $\xi_{30} = 1.616$ in system of Eqs. (16)–(23). Then we solved this system of eight equations (16)–(23) and found

$$a_1 = -0.250705, \qquad a_3 = -0.682679, \qquad a_4 = -0.598163,$$
$$a_6 = -0.824378, \qquad a_7 = -1.934379, \qquad a_8 = 3.959592,$$
$$\xi_{10} = \xi_{20} = 0.160159 \qquad (24)$$

Table 1. The dependence of some parameters (24) of the solution (10) on the meanings $\xi_{s,30}$ of ξ_{30}.

s	$\xi_{s,30} = \xi_{30} - s\xi_{30}$	a_1	a_8	ξ_{10}, ξ_{20}
0.000	1.6160	−0.2507	3.9595	0.1602
0.001	1.6144	−0.2253	−0.1767	3.9212
0.002	1.6128	−0.1677	−0.0714	4.3425

We verified the exactness of our approach considering the dependence of upper calculated parameters on the small changes of ξ_{30}. The results are presented in Table 1 and fast increasing of ξ_{10}, ξ_{20} for small decreasing of ξ_{30} values show that we used a very exact meaning $\xi_{30} = 1.616$ because ξ_{10}, ξ_{20} must be smaller than for diffusion in the plane [6].

2 Results and discussion

The less exact solution for three dimension case [5] where only linear terms in the expansion

$$f_A(\xi_1, \xi_2, \xi_3) = \sum_{i=1}^{3} a_i(\xi_i - \xi_{i0}) \tag{25}$$

were included gives following value for parameter $\xi_{30} = \sqrt{2}$ what is acceptable difference from our approximation $\xi_{30} = 1.616$. From here we can confirm that the terms R_3 in expansion (9) for our case are not important. Obtained approximate solution (10) sufficient exact and can be used for theoretical calculations of impurities spreading by diffusion from a square window in semiconductors by electronic devices processing. The experimental impurity profiles can be more exactly approximated [1] by solutions of nonlinear diffusion equation than by classical solutions [4] of linear diffusion equation where the fitting with the experimental profile tail region is important for exact modeling of integral micro schemes [5, 1]. Applications of solutions of linear diffusion equation for this case are impossible [3]. By dividing the diffusion coefficients on excitation parameter, we can apply obtained solution for nonisothermical diffusion [4] and diffusion in crystals excited [4] by irradiation [13]. Our results can also be used for the heat transfer problem from surfaces of materials heated with lasers [9, 12] because diffusion equation has the same form as heat transfer equation.

3 Conclusion

A handy approximate solution of nonlinear diffusion equation for three-dimensional case has been obtained. The obtained solution can be applied for evaluation of technological parameters for impurities introduction in semiconductors. The nonlinear diffusion equation and its solutions can be used for a more exact modeling of integral micro schemes production.

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REZIUMĖ

Netiesinės difuzijos lygties sprendinio modeliavimas trimačiu atveju

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Darbe gautas trimatės netiesinės difuzijos lygties apytikslis sprendinys, kai difuzijos koeficientai x, y ir z kryptimis yra proporcingi priemaišų koncentracijai. Trimatės netiesinės difuzijos lygties sprendinys išdėstomas trijų automodelinių kintamųjų laipsnine eilute maksimalaus priemaišų įsiskverbimo taškų x, y ir z aplinkose įskaitant kvadratinius narius. Gautas sprendinys naudingas praktiniuose taikymuose nustatant technologinius parametrus difuzijos procesams vykstant puslaidininkinių prietaisų gamyboje. Tai sudaro galimybę tiksliau modeliuoti integralines mikroschemas

Raktiniai žodžiai: netiesinė difuzijos lygtis, apytikslis sprendinys, automodelinis kintamasis.