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Nonlinear diffusivity dependence on dimensions

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Abstract. The nonlinear diffusion equation corresponds to the diffusion processes which can occur with a finite velocity. This statement is not satisfied in Fick's second law or linear diffusion equation. The processes by which different materials mix in the result of the random Brownian motions of atoms, molecules and ions can be exactly described only with presented nonlinear equation. It was important in practice that theoretically profiles fit with the experimental profiles tail region, but get good coincidence between diffusion experiments and the classical solutions is impossible. By using obtained theoretical solutions for two and three-dimensional cases we can provide more exact modeling of all the stages of a planar transistor formation.

Keywords: nonlinear diffusion equation, diffusion coefficients in higher dimensional, approximate analytical solution.

Introduction

In 1983, A.J. Janavičius proposed nonlinear diffusion equation which played an important role in theoretical and practical applications to technological processes of electronic devices and micro schemes [10, 14]. Here obtained approximate analytical solutions [14] were in good fitting with diffusion experiments in silicon. In 1984 M. Sapagovas with collaborators [3] considered nonlinear diffusion using numerical methods.The nonlinear theory accepted that diffusion processes must occur with finite velocity [1]. For this case diffusion coefficient must be directly proportional to the concentration of the impurities [5]. The equation was solved for excited atoms irradiated by X-rays and a new physical phenomenon such as impurities superdiffusion at room temperature in the crystals was found [2, 6] and verified experimentally [2]. We obtained important connections between higher dimensional and nonlinear diffusion coefficients and solutions by considering nonlinear diffusion through a square window in [4] two and three-dimensional cases. The root-mean-square displacement of the diffusion cloud [4]

$$\left\langle R_d^2 \right\rangle^{\frac{1}{2}} = \sqrt{2dD_d t}, \tag{1}$$

must be consented with Einstein expression for diffusion coefficient [4]

$$D_d = \frac{1}{2d} \Gamma_d \lambda^2. \tag{2}$$

Γ_d is diffusing particles jumping frequency in d dimensions, t is diffusion time. Statistical mechanics describes a sequence of unpredictable movement called a random walk. The rules of random walk can be simplified into one-dimensional random jumping of particles with constant frequencies. The displacements of particles after $n+1$-th jump of the length λ are

$$x_{n+1} = x_n \pm \lambda. \tag{3}$$

Taking both sides of this equation in square and overriding by a number of particles, requiring that the overage displacement $\langle x_n \rangle = 0$, we obtain

$$\langle x_{n+1}^2 \rangle = \langle x_n^2 \rangle + \lambda^2, \qquad \langle x_n^2 \rangle = N\lambda^2. \tag{4}$$

Accepting that the mean time τ of jumps of diffusing particles in the homogeneous matter must be constant for different stages of diffusion, we can get expression of the number of jumps $N = \frac{t}{\tau}$ for diffusion process duration time t. Then mean-square displacement and path of diffusion can be determined by

$$\langle x_n^2 \rangle = \lambda^2 \Gamma t, \qquad x_d = \sqrt{\langle x_n^2 \rangle} = \sqrt{\lambda^2 \Gamma t}. \tag{5}$$

If the particle is hoping in the random way the path of diffusion is proportional to the square root of the diffusion time. We can see that diffusion coefficient depends on frequency and length of jumps and geometry of task. The diffusion coefficients for diffusion in one D_1, two D_2 and three D_3 dimensional cases and paths of diffusion x_d can be expressed [4] in homogeneous environment

$$D_1 = \frac{1}{2}\lambda^2 \Gamma, \qquad D_2 = \frac{1}{4}\lambda^2 \Gamma, \qquad D_3 = \frac{1}{6}\lambda^2 \Gamma, \qquad x_d = \sqrt{2dD_d t}. \tag{6}$$

For a symmetric case of jumps' length λ, frequencies Γ of diffusing particles and diffusion path x_d does not depend on dimensions number. The diffusion coefficients $D = D_1$ for linear diffusion equation [4] for one-dimensional case

$$\frac{\partial}{\partial t} N = D \frac{\partial^2}{\partial x^2} N, \quad D = D_0 e^{-\frac{E}{kt}} \tag{7}$$

depend on exponential factor D_0, temperature T, Boltsmann's constants k and excitation energy E of diffusing atoms. The diffusion coefficient D for one-dimensional case in semiconductors can be defined from impurities profiles [5] or $p-n$ junctions' depths [8]. The experimental profile tail regions and theoretical solutions of linear diffusion equation cannot be fitted [10, 5]. The aim of the article is more exact definition of $p-n$ depths and thickness of planar diodes and transistors [8].

1 Nonlinear diffusion in one-dimensional case

The parameters of microelectronics can be sufficiently exactly defined by nonlinear diffusion equation [10] and impurities flux J [5] of thermodiffusion in silicon

$$\frac{\partial}{\partial t} N = \frac{\partial}{\partial x}\left(D(N) \frac{\partial}{\partial x} N \right), \qquad J = -D(N) \frac{\partial}{\partial x} N(x), \qquad D(N) = \frac{N(x)}{N_S} D. \tag{8}$$

The nonlinear diffusion coefficient is directly proportional to concentration of the impurities [10] and defined by impurities concentration N_S at the source. This model includes the physically realistic model according to which the impurities flux J, rewritten by the discretiation method [7], differs from zero at the point $x + \Delta x$ only if impurities are present at the point x. The latter equation means that the length of the jump of diffusing particles from the point x to $x + \Delta x$ in the diffusion process is not greater than Δx and the jump is possible only when a diffusing particle exists at the point x.

Now we will present a similarity solution [7] of the nonlinear diffusion equation (8) satisfying the boundary and initial conditions

$$N(0, t \geqslant 0) = N_S, \qquad N(\infty, t) = 0, \qquad N(x, 0) = 0, \quad x > 0. \tag{9}$$

Introducing the similarity variable [4]

$$\xi = \frac{x}{\sqrt{D_s t}}, \qquad D_s = D_n N_s, \qquad D_n = D(N) \tag{10}$$

and $N(x,t) = N_s f(\xi)$, into (8) we obtained equation for solution satisfying conditions (9)

$$2\frac{d}{d\xi}\left(f\frac{d}{d\xi}f\right) + \xi\frac{d}{d\xi}f = 0, \qquad f(\xi) = \sum_{n=0}^{m} a_n \xi^n, \quad a_0 = 1. \tag{11}$$

Then solution with included terms until fourth power $m = 4$ was expressed [5]

$$\begin{gathered} N_4 = N_s\bigl(1 - 0.44\xi - 0.098\xi^2 - 6.67 \times 10^{-3}\xi^3 + 4.002 \times 10^{-4}\xi^4\bigr), \\ \xi_{04} = 1.62, \qquad x_{04} = \xi_{04}\sqrt{N_S D_n t}, \quad 0 \leqslant x \leqslant x_{04}, \\ x_{04} = \xi_{04}\sqrt{D_S t}, \qquad D_S = N_S D_n. \end{gathered} \tag{12}$$

The obtained approximate solutions satisfy boundary and initial (9) conditions and sufficient good coincidence [3] with $\xi_0 = 1.64$. The obtained maximum penetration depths of impurities (12) are proportional to $\sqrt{t}$ and coincide with Brownian movement theory [4]. Substituting ξ_{04} into N_4 we got 1.71×10^{-3}, whence we see that the roots ξ_{04} and the solutions N_4 are obtained with sufficient accuracy.

2 Nonlinear diffusion in three-dimensional case

Rewriting equation (12) and using [2, 4] we obtained a nonlinear diffusion equation in the three-dimensional case

$$\frac{\partial}{\partial t}N = \frac{\partial}{\partial x}\left((D(N)\frac{\partial}{\partial x}N\right) + \frac{\partial}{\partial y}\left(D(N)\frac{\partial}{\partial y}N\right) + \frac{\partial}{\partial z}\left(D(N)\frac{\partial}{\partial z}N\right), \tag{13}$$

$$D(N) = \frac{1}{N_S}DN(x,y,z,t), \qquad N_2 = N(x,y,t), \qquad N_3 = N(x,y,z,t) \tag{14}$$

with diffusion coefficients $D(N)$ defined as $D(N_2)$ in the x, y plane and $D(N_3)$ according to z axe when off-diagonal elements equal zero [4]. Stochastic jumps of particles can occur according to orthogonal directions in the x, y and z axis. It can happen in crystals with diamond type lattice [4].

The equation (8) will be solved by introducing similarity variables [4]

$$\begin{gathered}
\xi_1 = \frac{|x| - h}{\sqrt{Dt}}, \qquad \xi_2 = \frac{|y| - h}{\sqrt{Dt}}, \qquad \xi_3 = \frac{z}{\sqrt{Dt}}, \\
h \leqslant |x| \leqslant x_0, \qquad h \leqslant |y| \leqslant y_0, \qquad 0 \leqslant z \leqslant z_0, \qquad z_0 = \xi_{30}\sqrt{Dt}, \\
0 \leqslant \xi_1 \leqslant \xi_{10}, \qquad 0 \leqslant \xi_2 \leqslant \xi_{20}, \qquad 0 \leqslant \xi_3 \leqslant \xi_{30}, \\
x_0 = \xi_{10}\sqrt{Dt} + h, \qquad y_0 = \xi_{20}\sqrt{Dt} + h,
\end{gathered} \tag{15}$$

for two-dimensional $N_2 = N(\xi_1, \xi_2)$ or three-dimensional case $N_3 = N(\xi_1, \xi_2, \xi_3)$ consequently describing the square source with the diagonals length $2h$ with defined corners (x_0, y_0) at $z = 0$.

For solution of (8) expressed in new similarity variables

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

$$\sum_{i=1}^{3} \left(2\frac{\partial}{\partial \xi_{id}} \left(f \frac{\partial f}{\partial \xi_{id}} \right) + \xi_{id} \frac{\partial f}{\partial \xi_{id}} + \xi_{i0} \frac{\partial f}{\partial \xi_{id}} \right) = 0, \tag{16}$$

$$\begin{gathered}
\xi_{1d} = \xi_1 - \xi_{10}, \qquad \xi_{2d} = \xi_2 - \xi_{20}, \qquad \xi_{3d} = \xi_3 - \xi_{30}, \\
-\xi_{10} \leqslant \xi_{1d} \leqslant 0, \qquad -\xi_{20} \leqslant \xi_{2d} \leqslant 0, \qquad -\xi_{30} \leqslant \xi_{3d} \leqslant 0,
\end{gathered} \tag{17}$$

we will use the approximate Taylor power expansion [7] at maximum penetration points ξ_{10}, ξ_{20}, ξ_{30} of impurities.

The solution $f(\xi_1, \xi_2, \xi_3)$ of (16) can be presented by the Taylor series by expansion [13]

$$\begin{aligned}
f(\xi_1, \xi_2, \xi_3) = f(P_0) &+ \sum_{i=1}^{3} (\xi_i - \xi_{i0}) \frac{\partial f}{\partial \xi_i}\bigg|_{P_0} + \frac{1}{2!} \sum_{i=1}^{3} \sum_{j=1}^{3} (\xi_i - \xi_{i0})(\xi_j - \xi_{j0}) \frac{\partial^2 f}{\partial \xi_i \partial \xi_j}\bigg|_{P_0} \\
&+ R_3.
\end{aligned} \tag{18}$$

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. Then we have

$$f(\xi_{1d}, \xi_{2d}, \xi_{3d}) = \sum_{i=1}^{3} \left(a_i \xi_{id} + a_{i+3} \xi_{id}^2 \right) + a_7 \xi_{1d} \xi_{2d} + a_8 \xi_{1d} \xi_{3d} + a_9 \xi_{2d} \xi_{3d}, \quad 0 \leqslant f \leqslant 1. \tag{19}$$

Substituting (19) into (16) and equating collected coefficients at ξ_{id}^n, with $n = 0, 1$; $i = 1, 2, 3$ to zero and using boundary conditions

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

$$f(0, -\xi_{20}, -\xi_{30}) = 0, \qquad \xi_1 = \xi_{10}, \quad \xi_2 = 0, \quad \xi_3 = 0, \tag{21}$$

$$f(-\xi_{10}, -\xi_{20}, 0) = 0, \qquad \xi_1 = 0, \quad \xi_2 = 0, \quad \xi_3 = \xi_{30}, \tag{22}$$

we define relative concentration of impurities in the center of the square (20) displaced in the x, y plane and zero concentration at the maximum penetration depths ξ_{10}, ξ_{20}, ξ_{30}, according to the coordinate axes x, y, z (21), (22) consequently. Then including the symmetry $f(\xi_1, \xi_2, \xi_3) = f(\xi_1, \xi_2, \xi_3)$ of solution for the square source (2) we obtained

$$\xi_{10} = \xi_{20}, \qquad a_1 = a_2, \qquad a_4 = a_5, \qquad a_8 = a_9. \tag{23}$$

Requiring that solution (19) must satisfy nonlinear equation (16) and boundary conditions (20), (21), (22) we got the following system of equations:

$$4a_1^2 + 2a_3^2 + 2\xi_{10}a_1 + \xi_{30}a_3 = 0, \tag{24}$$

$$a_1 + 16a_1a_4 + 4a_1a_7 + 4a_3a_8 + 4a_1a_6 + 2\xi_{10}a_4 + \xi_{30}a_8 + \xi_{10}a_7 = 0, \tag{25}$$

$$a_7 + 12a_4a_7 + 2a_6a_7 + 2a_8^2 = 0, \tag{26}$$

$$a_3 + 8a_1a_8 + 8a_3a_4 + 12a_3a_6 + 2\xi_{10}a_8 + 2\xi_{30}a_6 = 0, \tag{27}$$

$$a_8(1 + 8a_4 + 2a_7 + 6a_6) = 0, \tag{28}$$

$$-2a_1\xi_{10} - a_3\xi_{30} + 2a_4\xi_{10}^2 + a_6\xi_{30}^2 + a_7\xi_{10}^2 + 2a_8\xi_{10}\xi_{30} = 1, \tag{29}$$

$$-\xi_{10}a_1 - \xi_{30}a_3 + a_4\xi_{10}^2 + a_6\xi_{30}^2 + a_8\xi_{10}\xi_{30} = 0, \tag{30}$$

$$-2a_1 + 2\xi_{10}a_4 + \xi_{10}a_7 = 0. \tag{31}$$

The first five equations are obtained by equating the collected terms at constant, and at $(\xi_1-\xi_{10})$, $(\xi_1-\xi_{10})(\xi_2-\xi_{20})$, $(\xi_3-\xi_{30})$, $(\xi_1-\xi_{10})(\xi_3-\xi_{30})$ consequently. We got the last three equations (29), (30), (31) requiring to satisfy the boundary conditions (20)–(22). Equations we solved by using the computer algebra system Maple 14. The following meanings of constants for (19) was found

$$\begin{aligned} &a_1 = a_2 = 0, \quad a_3 = -0.745356, \quad a_4 = a_5 = -0.075000, \quad a_6 = -0.050000, \\ &a_7 = 0.150000, \quad a_8 = a_9 = 0, \quad \xi_{10} = \xi_{20} = 3.65148, \quad \xi_{30} = 1.49071. \end{aligned} \tag{32}$$

Then approximate solution of (19) can be represented

$$f(\xi_{1d}, \xi_{2d}, \xi_{3d}) = a_3\xi_{3d} + a_4\xi_{1d}^2 + a_4\xi_{2d}^2 + a_6\xi_{3d}^2. + a_7\xi_{1d}\xi_{2d}. \tag{33}$$

This solution does not satisfy conditions (6) for diffusion coefficients and paths for different dimensions. The presented results can be applied in inhomogeneous environment.

We can compare obtained solution with the same boundary conditions (14) using in power expansion essentially different variables $\xi_i^1 = \frac{\xi_i}{\xi_{i0}^1}$ until square terms were obtained as close solutions $\xi_{10}^1 = \xi_{20}^1 = 4$ and $\xi_{30}^1 = 1.42$. Here correlation term $\xi_1\xi_2$ as in (31) was not included and for this reason our solutions for ξ_{10}, ξ_{20}, ξ_{30} are more exact than values ξ_{10}^1, ξ_{20}^1, ξ_{30}^1. The terms $\xi_{30} = 1.49$ and $\xi_{30}^1 = 1.42$ coincide with sufficient accuracy.

Similar expansion in power series $(\xi - \xi_0)^n$ for solution of one-dimensional case of the nonlinear diffusion equation (11) gives the fast convergence of solution and maximum values ξ_{n0} for finite n [9]

$$\xi_{10} = \sqrt{2}, \qquad \xi_{20} = 1.633, \qquad \xi_{30} = 1.618, \qquad \xi_{40} = 1.616. \tag{34}$$

3 Results and conclusions

The obtained solutions (32), (33) are sufficiently exact and can be used for theoretical calculations of impurities spreading by diffusion from a square window in semiconductors for the production of electronic devices. The nonlinear diffusion equation for two-dimensional case also was solved [12] and the following result for maximum similarities variables was obtained $\xi_{10} = \xi_{20} = 0.429$.

Our results can also be used for the heat transfer problem in solids from surfaces of materials heated with lasers [11]. The presented nonlinear equation can be applied to gasses [1] and solid states.

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REZIUMĖ

Netiesinės difuzijos priklausomybė nuo dimensijų

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Straipsnyje nagrinėjami netiesinės difuzijos lygties sprendiniai vienmačiu ir trimačiu atvejais, pateikti maksimalūs priemaišų įsiskverbimo gyliai kietuose kūnuose. Nustatyti parametrai vienmačiam, dvimačiam ir trimačiam netiesinės difuzijos uždaviniui. Paprasto ryšio tarp difuzijos koeficientų kaip tiesinės difuzijos atveju negavome, bet yra galimybė pasirinkti prioritetines difuzijos sklidimo kryptis atsižvelgiant į kristalų struktūrą, aplinkos nehomogeniškumą.

Raktiniai žodžiai: netiesinė difuzijos lygtis, priemaišų įsiskverbimo gylis, difuzijos koefficientas, apytikslis analizinis sprendinys.