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# Nonlinear diffusion in three dimension case

Arvydas Juozapas JANAVIČIUS (ŠU)
*e-mail: yanavi@takas.lt*

## 1. Introduction

The classical linear diffusion equation can be derived from Fick's law or from the Fokker-Planck equation. In both cases were not included the restrictions that in the solids diffusion can ocure only by discrete steps and that process is slow. It is well known [1] that fitting an experimental tail region of impurities to classical solution $erfc\left(\frac{x}{\sqrt{2Dt}}\right)$ is impossible.

The presented nonlinear diffusion equation [2]

$$\frac{d}{dt}N = \frac{d}{dx}\left(D\cdot\frac{d}{dx}N\right), \quad j = -D\cdot\frac{d}{dx}N, \tag{1}$$

where the diffusion coefficient is directly proportional to the impurities concentration

$$D(t, N) = D_n\cdot N(x, t), \tag{2}$$

$$D_n = \frac{D_0}{N_s}\cdot e^{-\frac{E}{kT}}, \quad N_s = N(0, t) = const. \tag{3}$$

describes experimental profiles of impurities very well. Here, $D_0$ and $E$ are pre-exponential factor and activation energy, respectively. $N_s$ is constant surfice concentration of impurities.

## 2. Solution of the nonlinear diffusion equation in three dimension case

For the diffusion from the infinity source through the window we have the folowing boundary

$$N\left(0, 0\leqslant|y|\leqslant\frac{p}{2}, 0\leqslant|z|\leqslant\frac{a}{2}, t\right) = N_s, \quad N(\infty, \infty, \infty, t) = 0, \tag{4}$$

and initial

$$N\left(x > 0, |y|\geqslant\frac{p}{2}, |z|\geqslant\frac{a}{2}, 0\right) = 0 \tag{5}$$

conditions.

Introducing the similarities variables

$$\xi_1 = \frac{x}{\sqrt{D_s \cdot t}}, \quad \xi_2 = \frac{|y| - \frac{p}{2}}{\sqrt{D_s \cdot t}}, \quad \xi_3 = \frac{|z| - \frac{a}{2}}{\sqrt{D_s \cdot t}}, \quad D_s = D_n \cdot N_s, \qquad (6)$$

$$\xi_1 \geqslant 0, \qquad \xi_2 \geqslant 0, \qquad \xi_3 \geqslant 0$$

into the nonlinear equation

$$\frac{d}{dt} N = \frac{d}{dx}\left(D \cdot \frac{d}{dx} N\right) + \frac{d}{dy_1}\left(D \cdot \frac{d}{dy_1} N\right) + \frac{d}{dz_1}\left(D \cdot \frac{d}{dz_1} N\right), \qquad (7)$$

$$y_1 = |y|, \quad z_1 = |z|,$$

we get

$$\frac{d}{dt} f = \left[\sum_{i=1}^{3}\left(\frac{d}{d\xi_i} f \cdot \frac{d}{d\xi_i} f + \frac{1}{2} \cdot \xi_i \cdot \frac{d}{d\xi_i} f\right)\right], \qquad (8)$$

where

$$N = N_s \cdot f(\xi_1, \xi_2, \xi_3). \qquad (9)$$

$D_s$ is the diffusion coefficient which is equal to a constant.

In [3] was shown that solution of (8) with sufficient accuracy in one dimension case can be expressed using only first members of power series [3]. In three dimension case we use the same aproach

$$f = b_1 \cdot (\xi_1 - \xi_{01}) + b_2 \cdot (\xi_2 - \xi_{02}) + b_3 \cdot (\xi_3 - \xi_{03}). \qquad (10)$$

We shall find the solution in the region

$$0 \leqslant \xi_1 \leqslant \xi_{01}, \quad 0 \leqslant \xi_2 \leqslant \xi_{02}, \quad 0 \leqslant \xi_3 \leqslant \xi_{03}. \qquad (11)$$

For $b_2 = 0, b_3 = 0$ we must have diffusion in one dimension case. Then we have [3]

$$\xi_{01} = \sqrt{2}, \quad b_1 = -\frac{1}{\sqrt{2}}. \qquad (12)$$

Substituting (10) into (8) we get

$$b_1 + b_2 + b_3 = 0. \qquad (13)$$

Using initial and boundary conditions (4) and (5) we can get

$$f(0,0,0) = 1, \quad f(0, \xi_{02}, 0) = 0, \quad f(0, 0, \xi_{03}) = 0. \qquad (14)$$

From (10), (14) and (13) we get

$$b_2 = \frac{1}{2}\cdot\sqrt{2}, \quad b_3 = \frac{1}{2}\cdot\sqrt{2}, \quad \xi_{02} = \frac{1}{\sqrt{2}}, \quad \xi_{03} = \frac{1}{\sqrt{2}}. \tag{15}$$

The obtained solutions can be presented in following way

$$N = N_s\cdot\left[-\frac{1}{\sqrt{2}}\cdot(\xi_1 - \sqrt{2}) + \frac{1}{\sqrt{2}}\cdot\left(\xi_2 - \frac{1}{\sqrt{2}}\right) + \frac{1}{\sqrt{2}}\cdot\left(\xi_3 - \frac{1}{\sqrt{2}}\right)\right]. \tag{16}$$

The maxmimum penetration depth $\xi_{01}$ expressed in the similarity variables for $x$ direction equals $\sqrt{2}$. It coincides with mean-square displacement of the Brounian movement in one dimension case.

## 3. Conclusions

The obtained aproximate solution (16) can be used for the technologies of microelectronic devices and for finding the more exact aproaches, where must be used more members of power series than in (10). Then we must obtaine $\xi_{01} = 1.616$ like in one dimension case for more exact solutions [3].

## References

[1] A.N. Bubenikov, *Modeling of integral microtechnologies, devices and schemes*, High Scool, Moscow (1989).
[2] A.J. Janavičius, Method for solving the nonlinear diffusion equation, *Phys. Lett.* A224, 159–162 (1997).
[3] A.J. Janavičius, Ž. Norgėla, Problem of uniquenss of the physical solution of nonlinear diffusion equation, in: *Works of scientific seminar of Physics and mathematics facylty*, Šiaulių universitetas, 5–9 (1998).

# Netiesinė difuzija trimatėje erdvėje

A.J. Janavičius

Gautas apytikslis trimatės netiesinės difuzijos lygties sprendinys, tinkamas mikroelektronikos technologijoms. Šis sprendinys gali būti panaudotas gauti tikslesniems priartėjimams.