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Mathematical Modeling of Electric Potential in Semiconductors with Heterogeneous Dopant Profile

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Abstract

The theoretical modeling of electric field in semiconductors with heterogeneous doping profile has been done. The cases when electroconductivity changes with depth according to exponentional law or is described by Gaussian function have been considered. Theoretical justification has been giving by solving electrodynamic boundary value problem with certain boundary conditions. The expressions in the form of analytical function series for potential distribution at probe measurements have been obtained.

Keywords: heterogeneous semiconductor, boundary value problem, electric potential, probe measurement

1. Introduction

Semiconductors technologies realized on the base of semiconductor crystal and films are wildly used in modern electronics [1, 2]. More and more demanding requirements have been laid out for electric properties of such materials. The character of electric field distribution is really essential for practical usage of these materials and for the study of their properties.

With the help of different technological methods semiconductor films are produced in which the content of dopant impurity and electroconductivity correspondingly change with depth [1, 2]. In practice electoconductivity σ can change with depth according to exponentional law or be described by Gaussian distribution function [3-5].

In scientific literature there are examples of mathematical calculations of potential distribution in heterogeneous semiconductors with arbitrary doping profile [6]. The authors of the work describe [7] the technique of specific conductivity measurements for epitaxial and diffusional layers, which enable us to measure voltage at probe measurements using well-known laws describing impurity distribution with depth.

In work [8] the solution is found numerically for exponentional law of electroconductivity. The authors of these works calculated electroconductivity distribution analogically to the way they calculated multilayer structure with stepped distribution of charge carrier concentration. For each separate layer Laplace's equation is solved and then the obtained solutions are "sewn together" on the boundaries proceeding from the following conditions: potential continuity and normal component of current density. Similar techniques of electric field calculation are realized in some later works as applied to semiconductor films produced by modern methods [5, 9, 10].

However, the given solutions doesn't allow one to take into consideration the influence of the lateral boundaries of the sample, which makes their practical appliance more problematic. Numerical approximation of the method, described in work [8] implies error 6…27% (depending on the heterogeneity parameters), with the number of lays being equal to 51. It's not always possible to get the required convergence while doing the calculations with the expressions suggested in the work. Thus, there's still necessity to justify theoretically probe methods of semiconductor parameter measurements, taking into account the influence of sample boundary and a certain type of heterogeneity.

Our work is aimed at theoretical calculation of electric field distribution inside heterogeneous semiconductor at probe measurements, on the basis of which electric field is modeled in the region of the sample.

2. Mathematical Model of Potential Distribution

Let’s consider distribution of the electric field potential in heterogeneously doped semiconductor rectangular plate with geometrical dimensions *a*, *b* and *d*. Two current contacts are located on the surface of the sample (fig.1); (x_1, y_1), (x_2, y_2) are their coordinates.

In the case under the study plate electoconductivity changes with depth according to one of the following laws [3-5]:

$$\sigma_1(z) = \sigma_0 \exp(-2p\,z), \tag{1}$$

$$\sigma_2(z) = \sigma_0 \exp(-2\lambda\, z^2), \tag{2}$$

where σ_0 –surface elecrtroconductivity of the sample, *p* and λ – constant parameters, determined by the technology the heterogeneous lay was produced.

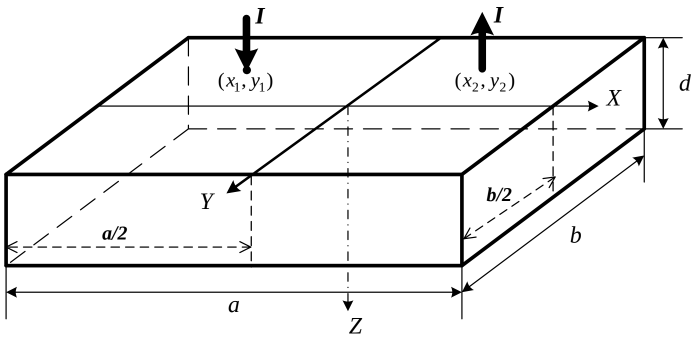


Fig.1 Schematic diagram of arrangement of current contacts on the heterogeneous sample.

For steady currents without charge sources and drain the following formulas are correct [11]:

$$\operatorname{div} \mathbf{j} = 0, \ \mathbf{j} = -\sigma \operatorname{grad} \varphi. \tag{3}$$

Consequently the potential of the electric field φ in the sample satisfies the equation:

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} + \frac{1}{\sigma(z)} \frac{\partial \varphi}{\partial z} \frac{\mathrm{d}\,\sigma(z)}{\mathrm{d}\, z} = 0. \tag{4}$$

We’ll get the boundary conditions from the requirement that normal component of electric current intensity is equal to zero everywhere on the sample surface except the points under the contact probes:

$$\left.\frac{\partial \varphi}{\partial z}\right|_{z=0} = -\frac{I}{\sigma_0 d}\left[\delta(x-x_1)\delta(y-y_1) - \delta(x-x_2)\delta(y-y_2)\right]; \tag{5}$$

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x=\pm a/2} = 0\,;\ \left.\frac{\partial \varphi}{\partial y}\right|_{y=\pm b/2} = 0\,;\ \left.\frac{\partial \varphi}{\partial z}\right|_{z=d} = 0\,. \tag{6}$$

Let’s represent the general solution of the problem (4-6) in the form of Fourier series:

$$\varphi(x,y,z) = \sum_{k,n=0}^{\infty}\left\{Z_{kn}(z)\cos\left[\alpha_k\,(x+a/2)\right]\cos\left[\beta_n\,(y+b/2)\right]\right\}, \tag{7}$$

where $\alpha_k = \pi k/a$, $\beta_n = \pi n/b$ (n,k=0,1,2…), $Z_{kn}(z)$ – a certain function, which will be identified later.

From formulae (1), (2) and (4) function $Z_{kn}^{(i)}(z)$ satisfies one of the equations:

$$\frac{\partial^2 Z_{kn}^{(1)}}{\partial z^2} - 2p\frac{\partial Z_{kn}^{(1)}}{\partial z} - \left(\alpha_k^2 + \alpha_n^2\right)Z_{kn}^{(1)} = 0\,, \tag{8}$$

$$\frac{\partial^2 Z_{kn}^{(2)}}{\partial z^2} - 4\lambda z\frac{\partial Z_{kn}^{(2)}}{\partial z} + \left(\alpha_k^2 + \alpha_n^2\right)Z_{kn}^{(2)} = 0\,, \tag{9}$$

where index i=1 is referred to exponential law, and index i=2 is referred to Gauss's law, describing the change of electroconductivity with depth.

After substituting boundary conditions (5), (6) and after doing necessary transformations we obtained general expression of potential distribution $\varphi^{(1)}$ in the sample for the situation when electroconductivity of the sample changed with depth according to exponential law (1):

$$\varphi^{(1)}(x,y,z) = \frac{4I}{ab\sigma_0}\sum_{n,k=0}^{\infty}\left\{A_{kn}\left[\frac{e^{(p-\eta_{kn})z}}{(\eta_{kn}-p)\cdot(e^{-2\eta_{kn}d}-1)} + \frac{e^{(p+\eta_{kn})z}}{(\eta_{kn}+p)\cdot(1-e^{2\eta_{kn}d})}\right]\times \cos\left[\alpha_k\left(x+\frac{a}{2}\right)\right]\cos\left[\beta_n\left(y+\frac{b}{2}\right)\right]\right\}, \tag{10}$$

where

$$A_{kn} = \Theta_{kn}\left(\cos\left[\alpha_k\left(x_1+\frac{a}{2}\right)\right]\cos\left[\beta_n\left(y_1+\frac{b}{2}\right)\right] - \cos\left[\alpha_k\left(x_2+\frac{a}{2}\right)\right]\cos\left[\beta_n\left(y_2+\frac{b}{2}\right)\right]\right), \tag{11}$$

$$\eta_{kn} = \sqrt{p^2 + \alpha_k^2 + \beta_n^2}\,,\ \Theta_{kn} = \begin{cases} 0, & \text{for } n = k = 0; \\ 0.5, & \text{for } n = 0, k \neq 0 \text{ or } k = 0, n \neq 0; \\ 1, & \text{for } n \neq 0, k \neq 0. \end{cases} \tag{12}$$

In the case when electroconductivity changes with depth according to the Gaussian distribution function (2), the expression for potential in the sample $\varphi^{(2)}$ acquires the form:

$$\varphi^{(2)}(x, y, z) = \frac{4I}{ab\sigma_0} \sum_{n,k=0}^{\infty} \left\{ A_{kn} \left(z\ \Phi\left(q + \frac{1}{2}; \frac{3}{2}; 2\lambda z^2 \right) - C_{kn} \frac{\Phi(q; 1/2; 2\lambda z^2)}{\alpha_k^2 + \beta_n^2} \right) \times \right. \\ \left. \cos\left[\alpha_k \left(x + \frac{a}{2} \right) \right] \cos\left[\beta_n \left(y + \frac{b}{2} \right) \right] \right\}, \tag{13}$$

where

$$q = \frac{\alpha_k^2 + \beta_n^2}{8\lambda}\,,\ C_{kn} = \frac{3\Phi(q + 1/2; 3/2; 2\lambda d^2) + 8\lambda d^2 [q + 1/2] \cdot \Phi(q + 3/2; 5/2; 2\lambda d^2)}{3d\ \Phi(q + 1; 3/2; 2\lambda d^2)}\,, \tag{14}$$

$\Phi(t_1; t_2; t_3)$ – Kummer's function (confluent hypergeometric function) [12, 13].

In case of homogeneous semiconductor (p=λ=0) the obtained expressions for the potentials (10), (13) coincide with the solution described in the literature [14, 15] and can be presented in the following form:

$$\varphi^{(0)}(x, y, z) = \frac{4I}{ab\sigma_0} \sum_{n,k=0}^{\infty} \left\{ A_{kn} \frac{\mathrm{ch}(\xi_{nk}(z - d))}{\xi_{nk}\mathrm{sh}(\xi_{nk} d)} \cos\left[\alpha_k \left(x + \frac{a}{2} \right) \right] \cos\left[\beta_n \left(y + \frac{b}{2} \right) \right] \right\}, \tag{15}$$

where $\xi_{kn} = \sqrt{\alpha_k^2 + \beta_n^2}$.

3. Computer Modelling and Analysis of the Results

On the basis of the obtained calculating formula (10) calculated equipotential surfaces for the sample with the following relative parameters *b/a*=1, *d/a*=0.01; x_1=-0.4*a*, x_2=0.4*a*, y_1=y_2=0 are the coordinates of the current probes. The potential distribution is built using the program MathCAD [16]. The result of the of equipotential surface calculation in XY plane and in XZ plane for homogeneous sample is represented in Fig. 2.a While doing the calculations we had to sum up Fourier series up to 400 items for each index to have calculation error not more than 2%. In the figures presented below metric scales along the 0*x* axis and 0z axis don't coincide, this helps to present the results more vividly.

The result of equipotential surfaces constructing on the cut in XY plane and in XZ plane for heterogeneous sample the electroconductivity of which changes within depth according to equipotential law (1) is presented in fig.2 (for the following parameters of heterogeneity p=10/a (b), p=10^2/a (c), p=10^4/a (d)).

We also have constructed equipotential surfaces on the cut in XY plane and in XZ plane for heterogeneous sample the electroconductivity of which changes within depth according to Gauss's law (fig.3).The following parameters were chosen while modeling: $\lambda=10a^{-2}$ (a), $\lambda=10^4a^{-2}$ (b).

The results of the modelling show that potential distribution changes considerably with the change in heterogeneity parameters (p or λ). The constructed electric field models demonstrate that we have more homogeneous potential distribution in the sample by its depth as well as in plane of contacts with the rise in heterogeneity parameters (p or λ).

The results of the given calculations may serve a theoretical basis for practical development of probe express-methods aimed at calculating the parameters of heterogeneously doped semiconductors. The obtained expressions for electric field modeling can present certain interest for those who develop electronic technologies and need to optimize the distribution of heat and charge flow in microelectronic and nanoelectronic elements.

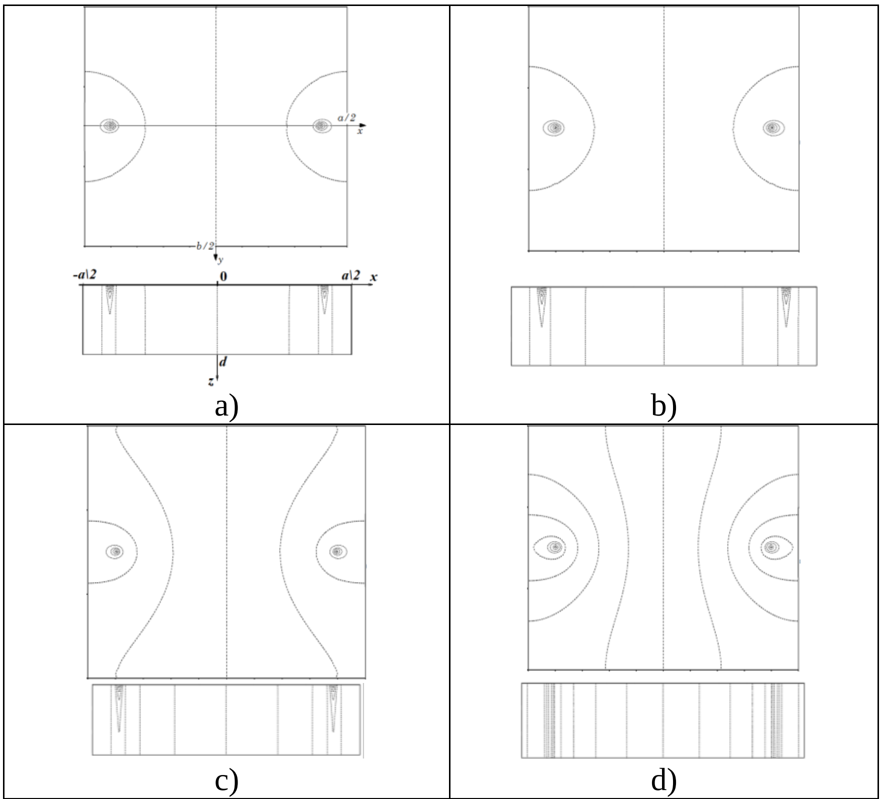
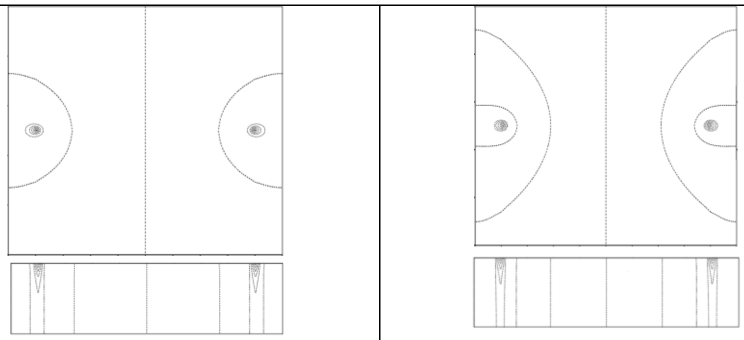


Fig. 2 Equipotential line distribution in heterogeneous semiconductor, for the heterogeneity when $\sigma_1(z) = \sigma_0 \exp(-2pz)$.



a) b)

Fig. 3 Equipotential line distribution in heterogeneous semiconductor, for the heterogeneity when $\sigma_2(z) = \sigma_0 \exp(-2\lambda z^2)$.

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