Improved diffusion-equation finite difference schema in numerical solution of the nonlinear Poisson equation

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Abstract **In this work a numerical iterative method for solving the nonlinear Poisson equation has been developed with the use of the diffusion-equation (parabolic) finite difference schema, to describe semiconductor hetero-structures. Procedures to control the convergence and stability of the method are presented. The approach enables us to solve the nonlinear Poisson equation in a small number of iterations, regardless of the level of hetero-structure complexity, type of electrical contacts and passive dielectric layers. Some numerical results obtained by this method for nBn Hg$_{1-x}$Cd$_x$Te hetero-structure infrared detectors with metal contacts are reported**.

I Introduction

The numerical modelling of semiconductor devices is usually based on four coupled differential equations: the Poisson equation, electron and hole balance equations (called current continuity equations) and energy balance equation. All these four equations are non-linear. The Poisson equation can be solved separately in the case of thermal equilibrium, which is the first step to consider the non-equilibrium phenomena. A stable numerical procedure for approximate solving it is needed. An approach commonly used is based on applying Newton's method for the discretised equation. Two features of the numerical method are then especially important: the suitable choice of initial values of electrical potential and the stability of iterative algorithms. In [1] A. Jóźwikowska has proposed an iterative numerical method for solving the nonlinear Poisson equation for semiconductor devices with the application of the diffusion-equation finite difference schema. In this method the non-linear Poisson equation was replaced by an equivalent diffusion equation which was solved to achieve a stationary state approximately. The method was pretty stable and applicable regardless of the level of hetero-structure complexity, type of electrical contacts and passive dielectric layers. Stability conditions were not defined precisely. In this paper we have improved this method by adding a heuristic approach to obtain the optimal values of pseudo-time step. This allows for the significant reduction of the number of iterations,

increasing the efficiency of the method. The Poisson equation can be represented in the following form:

$$\varepsilon_0 \nabla(\varepsilon \nabla \Psi) + e\rho = 0, \quad (1)$$

where $\rho(\Psi) = p(\Psi) - n(\Psi) + N_D^+(\Psi) - N_A^-(\Psi)$ is the electric charge density equal to the difference between the densities of positive and negative charge carriers (hole concentration plus concentration of ionized donors minus electron concentration and minus concentration of ionized acceptors); ∇ is the Hamilton differential operator. Eq. (1) is nonlinear due to the nonlinear dependence of the charge density on the potential. A method for finding the potential Ψ from Eq. (1) with boundary conditions, used in this work, relies on substituting (1) for diffusion (parabolic) equation

$$\frac{\partial \Psi}{\partial t} = \varepsilon_0 \nabla(\varepsilon \nabla \Psi) + e\rho, \quad (2)$$

with pseudo-time (dimensionless) variable t added. Given boundary conditions fixed and an initial guess for Ψ, Eq. (2) is solved until $\frac{\partial \Psi}{\partial t} = 0$ (approximately). In this way the process of solving (2) can be interpreted as the transition from the initial (non-equilibrium) electrostatic potential distribution to a stationary state enforced by boundary condition. The computations are performed with a discrete approximation of Eq. (2). The construction of corresponding finite difference schema is explained in this paper in detail for an infrared detector structure. As an example, let us consider mesa cylindrical structure of HgCdTe nBn infrared detector presented in Fig. 1. The device consists of a four-layer (n$^+$-B-n-N$^+$) structure deposited on the CdTe buffer layer .
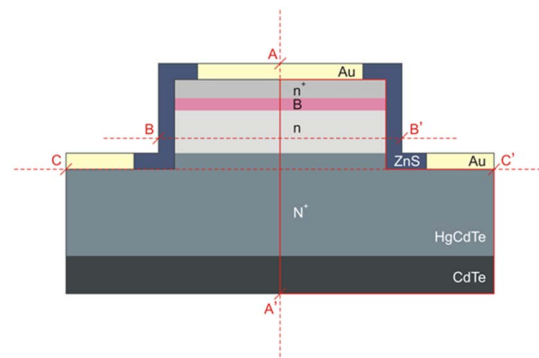

Fig. 1. The cross-section of HgCdTe mesa structure.
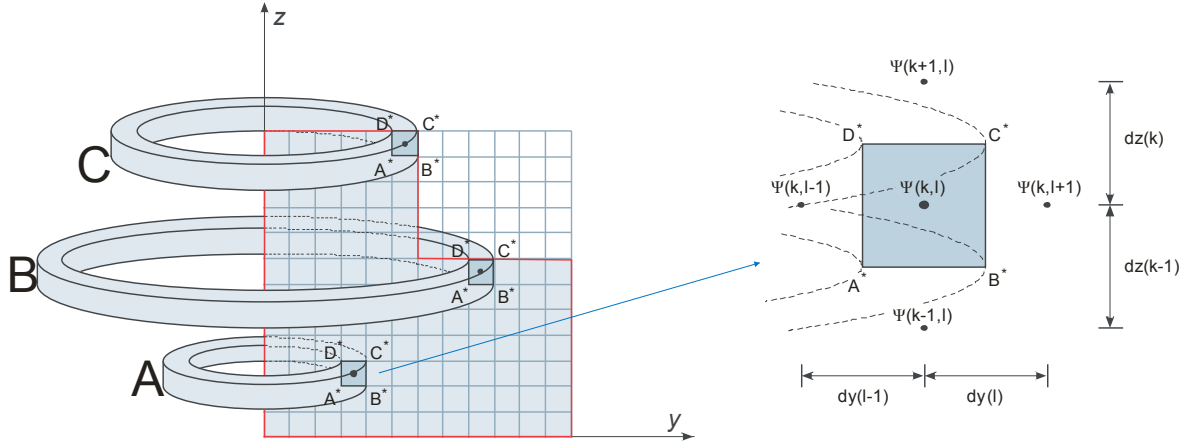
II COMPUTATION METHOD

Fig. 2. Definition of two-dimensional finite difference mesh. The coloured area states for half axial cross-section of the device from figure 1. The analyzed structure is divided into rings with rectangular cross sections $A^*B^*C^*D^*$ around each mesh point in the centre. The values of electrical potential are to be computed in central points. The rings are divided into three classes with respect to a number of faces being parts of external faces of the device: none (A), one (B) or two (C).

To construct the numerical method and perform computations the device shown in Fig. 1 (axially symmetric cylindrical) are divided into toroidal rings with rectangular cross sections defining the mesh for two-dimensional finite difference schema (Fig. 2) in the axial cross section of the analysed structure. The rings are considered in semiconductor domains as well as in metallic contacts and dielectric layers (Ref. [1]). The rings can be divided into three different classes with respect to a number of faces being parts of external faces of the device (Fig. 2): none (A), one (B) or two (C). We have obtained the numerical equation

$$\frac{\Psi^{n+1}(k,l) - \Psi^{nLAX}(k,l)}{\Delta t} = L(\Psi^n) \quad (3)$$

which approximately substitutes Eq. (2), with finite-difference operator

$$
\begin{aligned}
L(\Psi^n) &= A \frac{\varepsilon(k, l-1)\beta(l)}{\varepsilon(k, l-1)\beta(l) + \varepsilon(k,l)\beta(l-1)} [\Psi^n(k, l-1) \\
&\quad - \Psi^n(k,l)] \\
&+ B \frac{\varepsilon(k, l+1)\beta(l)}{\varepsilon(k, l+1)\beta(l) + \varepsilon(k,l)\beta(l+1)} [\Psi^n(k, l+1) \\
&\quad - \Psi^n(k,l)] \\
&+ C \frac{\varepsilon(k+1, l)\gamma(k)}{\varepsilon(k+1, l)\gamma(k) + \varepsilon(k,l)\gamma(k+1)} [\Psi^n(k+1, l) \\
&\quad - \Psi^n(k,l)] \\
&+ C \frac{\varepsilon(k-1, l)\gamma(k)}{\varepsilon(k-1, l)\gamma(k) + \varepsilon(k,l)\gamma(k-1)} [\Psi^n(k-1, l) \\
&\quad - \Psi^n(k,l)] \\
&+ e\{p(k,l) - n(k,l) + N_D^+(k,l) \\
&\quad - N_A^-(k,l)\} \quad (4)
\end{aligned}
$$

$R(l)$ is the mean radius of considered toroidal ring

$$A = \frac{[R(l)-0.5\beta(l)]\varepsilon_0\varepsilon(k,l)}{R(l)[\beta(l)]^2}, \qquad B = \frac{[R(l)+0.5\beta(l)]\varepsilon_0\varepsilon(k,l)}{R(l)[\beta(l)]^2}, \qquad C = \frac{\varepsilon_0\varepsilon(k,l)}{[\gamma(k)]^2} \cdot \beta(l+1) + \beta(l) = dy(l+1), \gamma(k+1) + \gamma(k) = dz(k+1), \gamma(k-1) + \gamma(k) = dz(k), \text{ and } \Psi(k,l)^{LAX} = \frac{1}{4}(\Psi_1 + \Psi_2 + \Psi_3 + \Psi_4),$$ where

$$\Psi_1 = \frac{\Psi(k,l-1)\varepsilon(k,l-1)\beta(l)+\Psi(k,l)\varepsilon(k,l)\beta(l-1)}{\varepsilon(k,l-1)\beta(l)+\varepsilon(k,l)\beta(l-1)}.$$

$$\Psi_2 = \frac{\Psi(k,l+1)\varepsilon(k,l+1)\beta(l)+\Psi(k,l)\varepsilon(k,l)\beta(l+1)}{\varepsilon(k,l+1)\beta(l)+\varepsilon(k,l)\beta(l+1)}$$

$$\Psi_3 = \frac{\Psi(k+1,l)\varepsilon(k+1,l)\gamma(k)+\Psi(k,l)\varepsilon(k,l)\gamma(k+1)}{\varepsilon(k+1,l)\gamma(k)+\varepsilon(k,l)\gamma(k+1)},$$

$$\Psi_4 = \frac{\Psi(k-1,l)\varepsilon(k-1,l)\gamma(k)+\Psi(k,l)\varepsilon(k,l)\gamma(k-1)}{\varepsilon(k-1,l)\gamma(k)+\varepsilon(k,l)\gamma(k-1)},$$
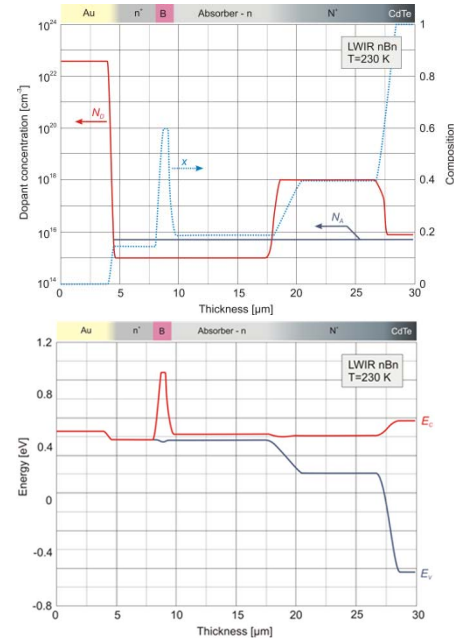

Fig. 3. Theoretical assumption of composition and dopant profiles along A-A' cross section (Fig. 1) of LWIR HgCdTe nBn detector.

Fig.4. . Calculated energy band diagram along A-A' cross section (Fig. 1) of LWIR HgCdTe nBn detector with a zero valence band offset.

REFERENCES

[1] A. Jóźwikowska, "Numerical solution of the nonlinear Poisson equation for semiconductor devices by application of a diffusion-equation finite difference scheme," *J. Appl. Phys.* 104, 063715,2008.