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MODELING OF SILICON DIFFUSION IN GALLIUM ARSENIDE.
3. NUMERICAL METHOD FOR SOLVING THE DIFFUSION EQUATION

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A finite-difference approximation is obtained and investigated and an algorithm for numerical solution of the diffusion equation for silicon atoms in gallium arsenide is constructed.

Having developed a model of the transition of impurity atoms between sublattices of gallium arsenide [1] and a model of solid-phase silicon diffusion [2], we will formulate an algorithm for numerical solution of the diffusion equation for silicon atoms.

First, we will construct a finite-difference approximation of diffusion equation (3) from [2]. To do this, using expressions (13) and (14) obtained in [2] for the transfer coefficients, we will evaluate $D-\chi R$:

$$D-\chi R=D_i(1-\beta_2\chi^2-2\beta_3\chi^3-3\beta_4\chi^4)/\beta_0\,. \qquad (1)$$

Integrating (1) with respect to χ, we will represent Eq. (3) from [2] as follows:

$$C_t^T=L_1\psi+L_2\psi\,, \qquad (2)$$

$$L_1\varphi=\Delta\,(D\,(\chi)\,\widetilde{C}_{\mathrm{Ga}}^{V\times}\,C)\,, \qquad (3)$$

$$L_2\psi=\nabla\,(\mu\,\nabla\,H)\,, \qquad (4)$$

$$\mu=\omega^{\chi}\,\widetilde{C}_{\mathrm{Ga}}^{V\times}\,(C/\chi)\,, \qquad (5)$$

$$H\,(\chi)=D_i\left(\chi-\frac{1}{3}\beta_2\chi^3-\frac{1}{2}\beta_3\chi^4-\frac{3}{5}\beta_4\chi^5\right)/\beta_0\,. \qquad (6)$$

We will introduce a grid for the time variable t with the nodes $\{t^j\}$ ($j=1, 2, ..., m$) and an ordinary uniform grid for the space variables. Assume that t^j and t^{j+1} correspond to t and $\hat{t}$ for the chosen j. Using the balance method and averaging the nonlinear terms in the right-hand side of (2) over the range of variation of the exact solution, we obtain a difference scheme of the form

$$\frac{\widetilde{C}^T-C^T}{\hat{t}-t}=\Lambda_1\,\varphi_I+\Lambda_2\,\psi_I\,, \qquad (7)$$

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$$\varphi_I = \frac{1}{\hat{C} - C} \int\limits_{C}^{\hat{C}} \varphi(C)\, dC, \tag{8}$$

$$\psi_I = \frac{1}{\hat{C} - C} \int\limits_{C}^{\hat{C}} \psi(C)\, dC, \tag{9}$$

$$\hat{C}^T = C^T(x, \hat{t}), \quad C^T = C^T(x, t), \quad \hat{C} = C(x, \hat{t}), \quad C = C(x, t), \tag{10}$$

where the difference operators Λ_1, Λ_2 approximate the operators L_1, L_2 on the uniform grid with second-order accuracy [3].

As follows from [4], not only the conservatism condition but also an additional energetic relation, valid for the initial differential model and having a certain physical meaning, will be fulfilled for Eq. (7). The absence of discrete disbalances in the grid analog of the conservation law provides a high efficiency for these schemes in "crude" grid computations of singularity problems as well as in calculations on large time intervals. The efficiency of this method in modeling arsenic diffusion in silicon and also in solving two-dimensional problems is demonstrated in [5].

We will dwell in more detail on techniques for evaluating integrals (8) and (9). Using various closed-type Newton-Cothes formulas [6], we can obtain a whole set of difference schemes for Eq. (7). In the present work we will consider the simplest integration formulas, namely, the trapezium formula and Simpson's formula. Combining these two formulas into one expression gives

$$\varphi_I = \frac{\delta}{6}(\varphi + 4\bar{\delta}\,\bar{\varphi} + \hat{\varphi}), \tag{11}$$

$$\varphi = \varphi(C), \quad \bar{\varphi} = \varphi(\bar{C}), \quad \hat{\varphi} = \varphi(\hat{C}), \tag{12}$$

$$\bar{C} = (C + \hat{C})/2, \tag{13}$$

$$\psi_I = \frac{\delta}{6}(\psi + 4\bar{\delta}\,\bar{\psi} + \hat{\psi}), \tag{14}$$

$$\psi = \psi(C), \quad \bar{\psi} = \psi(\bar{C}), \quad \hat{\psi} = \psi(\hat{C}). \tag{15}$$

As can be seen from (11)-(15), for $\delta = 3$, $\bar{\delta} = 0$ we obtain the trapezium formula, and for $\delta = 1$, $\bar{\delta} = 1$, the Simpson formula. The error ε_I in evaluating integral (8) by the trapezium and Simpson's methods is, respectively,

$$\varepsilon_I = \frac{(\hat{C} - C)^2}{12} \varphi''(\zeta), \quad C < \zeta < \hat{C} \tag{16}$$

and

$$\varepsilon_I = \frac{(\hat{C} - C)^4}{2880} \varphi^{(4)}(\zeta), \quad C < \zeta < \hat{C}. \tag{17}$$

Similar estimates are found for integral (9) as well.

It should be noted that if the transition of silicon into nodes of the arsenic sublattice is neglected, then at large impurity concentrations $C >> n_i$ it can be written that

$$\chi \approx C/n_i, \tag{18}$$

$$D(\chi) \approx D_i\,[1 + \beta_1 C/n_i + \beta_2 (C/n_i)^2 + \beta_3 (C/n_i)^3 + \beta_4 (C/n_i)^4]/\beta_0 . \tag{19}$$

This means that with a homogeneous distribution of neutral vacancies of gallium ($\widetilde{C}_{\mathrm{Ga}}^{V\times} = 1$) the following expression holds for the function φ:

$$\varphi \approx D_i\,[C + \beta_1 C^2/n_i + \beta_2 C^3/n_i^2 + \beta_3 C^4/n_i^3 + \beta_4 C^5/n_i^4]/\beta_0 , \tag{20}$$

i.e., the function φ is a fifth-power polynomial in C. This means that if an integration formula of higher accuracy is used to calculate (8), for example, Bode's formula [6]

$$\varphi_I = \frac{1}{90}\,(7\varphi + 32\varphi_1 + 12\overline{\varphi} + 32\varphi_2 + 7\widehat{\varphi}) , \tag{21}$$

$$\varphi_1 = \varphi\,(3C/4 + \widehat{C}/4) , \quad \varphi_2 = \varphi\,(3\widehat{C}/4 + C/4) , \tag{22}$$

then the value will be calculated accurately because the error is

$$\varepsilon_I = \frac{(\widehat{C} - C)^6}{1935360}\,\varphi^{(6)}(\zeta) \equiv 0 , \tag{23}$$

Now it will be assumed that the impurity atoms are transferred by threefold charged intrinsic point defects, i.e., $\beta_1 = \beta_2 = \beta_4 = 0$, $\beta_3 \neq 0$. Then for large C

$$\varphi \approx D_i\,(C + \beta_3 C^4/n_i^3)/\beta_0 , \tag{24}$$

and the error is equal to

$$\varepsilon_I = \frac{D_i \beta_3}{\beta_0\, n_i}\left(\frac{\zeta}{n_i}\right)^4 (\widehat{C} - C)^2 \tag{25}$$

in integration by the trapezium method and to

$$\varepsilon_I = \frac{D_i \beta_3}{120\,\beta_0\, n_i^3}\,(\widehat{C} - C)^4 \tag{26}$$

in integration by Simpson's method. It should be taken into consideration that for a typical diffusion process the characteristic value is $n_i \sim 10^5\,\mu\mathrm{m}^{-3}$, and $(\zeta/n_i) < 50$. From expressions (25) and (26) it is seen that with Simpson's method the required integration accuracy will be achieved even at high values of $(\widehat{C} - C)$, i.e., at large time steps, whereas with integration by the trapesium method the time step should be sufficiently small. The result obtained will also be valid in the case where transitions of silicon atoms into nodes of the arsenic sublattice are taken into account, because in this case the nonlinearity of the effective diffusivity of the impurity $D(\chi)$ decreases.

Substitution of expressions (11) and (14) into (7) transforms this equation into

$$\frac{\widehat{C}^T - C^T}{\widehat{t} - t} = \frac{\delta}{6}\,\Lambda_1\,(\varphi + 4\bar{\delta}\,\overline{\varphi} + \widehat{\varphi}) + \frac{\delta}{6}\,\Lambda_2\,(\psi + 4\bar{\delta}\,\overline{\psi} + \widehat{\psi}) . \tag{27}$$

In the one-dimensional case on the grid $\overline{\omega}_h = \{x_i = ih,\ i = \overline{0, m_x}\}$ with account for (3) and (4) the difference scheme of second order of accuracy will be as follows:

$$\frac{\widehat{C}^T - C^T}{\widehat{t} - t} = \frac{\delta}{6}\,(\varphi + 4\bar{\delta}\,\overline{\varphi} + \widehat{\varphi})_{xx} + \frac{\delta}{6}\,(\mu H_x + 4\bar{\delta}\,\overline{\mu}\,\overline{H}_x + \widehat{\mu}\,\widehat{H}_x)_x , \tag{28}$$

$$\mu = \mu\,(C)\,, \quad \overline{\mu} = \mu\,(\,\overline{C}\,)\,, \quad \widehat{\mu} = \mu\,(\,\widehat{C}\,)\,, \tag{29}$$

$$H = H\,(C)\,, \quad \overline{H} = H\,(\,\overline{C}\,)\,, \quad \widehat{H} = H\,(\,\widehat{C}\,)\,, \tag{30}$$

or in index form

$$\begin{gathered}
\frac{\widehat{C}_i^{\,T} - C_i^T}{\widehat{t} - t} = \frac{\delta}{6}\,(\varphi + 4\overline{\delta}\,\overline{\varphi} + \widehat{\varphi}\,)_{x\overline{x}} + \frac{\delta}{12\,h^2}\,(\mu_{i+1}\,\psi_{i+1} + \mu_i\,\psi_{i+1} - \\
- \mu_{i+1}\,\psi_i - 2\,\mu_i\,\psi_i - \mu_{i-1}\,\psi_i + \mu_i\,\psi_{i-1} + \mu_{i-1}\,\psi_{i-1} + 4\overline{\delta}\,(\,\overline{\mu}_{i+1}\,\overline{\psi}_{i+1} + \\
+ \overline{\mu}_i\,\overline{\psi}_{i+1} - \overline{\mu}_{i+1}\,\overline{\psi}_i - 2\,\overline{\mu}_i\,\overline{\psi}_i - \overline{\mu}_{i-1}\,\overline{\psi}_i + \overline{\mu}_i\,\overline{\psi}_{i-1} + \overline{\mu}_{i-1}\,\overline{\psi}_{i-1}) + \\
+ \widehat{\mu}_{i+1}\,\widehat{\psi}_{i+1} + \widehat{\mu}_i\,\widehat{\psi}_{i+1} - \widehat{\mu}_{i+1}\,\widehat{\psi}_i - 2\,\widehat{\mu}_i\,\widehat{\psi}_i - \widehat{\mu}_{i-1}\,\widehat{\psi}_i + \\
+ \widehat{\mu}_i\,\widehat{\psi}_{i-1} + \widehat{\mu}_{i-1}\,\widehat{\psi}_{i-1}\,]\,, \quad i = 1\,,\,2\,,\,\ldots\,,\,m_x\,.
\end{gathered} \tag{31}$$

System of equations (31) ia a system of nonlinear algebraic equations with a three-diagonal matrix relative to the unknowns $\widehat{C}_{i-1}$, $\widehat{C}_i$, and $\widehat{C}_{i+1}$. These values were found with Newton's linearization of (31) [3]. The resultant linear three-point equation has the form

$$A_i^k\,\widehat{C}_{i-1}^{k+1} + B_i^k\,\widehat{C}_i^{k+1} + C_i^k\,\widehat{C}_{i+1}^{k+1} = F_i^k\,, \quad i = 1\,,\,2\,,\,\ldots\,,\,m_x\,, \tag{32}$$

where A_i^k, B_i^k, C_i^k, and F_i^k are the coefficients and the free term of Eq. (32), calculated with the use of $\widehat{C}_{i-1}^k$, $\widehat{C}_i^k$, and $\widehat{C}_{i+1}^k$, determined in the previous iteration. The factorization method [3] was used to solve system of equations (32); the required solution of system (32) was obtained by iteration in k.

Now we will consider the construction of boundary conditions for (2). As follows from (2), the flow of impurity atoms is determined by the expression

$$j = -\,(\nabla\varphi + \mu\nabla H)\,. \tag{33}$$

We will consider the one-dimensional case and prescribe the boundary conditions in the most general form:

$$W_1\,(\varphi_x + \mu H_x)\,|_{x=0} + W_2 C\,|_{x=0} = W_3\,, \tag{34}$$

$$W_4\,(\varphi_x + \mu H_x)\,|_{x=x_F} + W_5 C\,|_{x=x_F} = W_6\,. \tag{35}$$

As one can see from (33) and (34), depending on the values of the parameters W_1 and W_2 at the left boundary, we can prescribe boundary conditions of the first ($W_1 = 0$, $W_2 = 1$), second ($W_1 = 1$, $W_2 = 0$), or third kind ($W_1 \neq 0$, $W_2 \neq 0$). Similarly, at the right boundary $x = x_F$ at $W_4 = 0$, $W_5 = 1$, we have boundary conditions of the first, at $W_4 = 1$, $W_5 = 0$, of the second, and at $W_4 \neq 0$, $W_5 \neq 0$, of the third kind.

For the finite-difference approximation of conditions (34) and (35) use is made of the method of fictitious regions. For this purpose it is assumed that the semiconductor medium extends fictitiously beyond its surface into the region $x < 0$ and extends into the region $x > x_F$. The fictitious node $i = 0$, positioned at the distance h from the semiconductor surface, will be introduced into the region $x < 0$ and it will be assumed that the fictitious value of the concentration at this node is equal to $\widehat{C}_0$. The characteristics of the medium in this region, including the distribution of defects, are assumed to be similar to the electrophysical parameters in the region [$i = 1$, $i = 2$], i.e., $\widetilde{C}_{\mathrm{Ga}_0}^{V\times} = \widetilde{C}_{\mathrm{Ga}_2}^{V\times}$; $N_0 = N_2$; $A_0 = A_2$. Then, we approximate boundary condition (34) with second order of accuracy with respect to x. The finite-difference scheme obtained takes the following form:

$$W_1 \left[\frac{\hat{\varphi}_2 - \hat{\varphi}_0}{2h} + \hat{\mu}_1 \frac{\hat{H}_2 - \hat{H}_0}{2h} \right] + W_2 \hat{C}_1 = W_3 , \tag{36}$$

$$\hat{\varphi}_0 = D(\hat{\chi}_0)\, \hat{\hat{C}}^{V\times}_{\mathrm{Ga}_0}\, \hat{C}_0 , \tag{37}$$

$$\hat{H}_0(\chi) = D_i \left(\hat{\chi}_0 - \frac{1}{3}\beta_2 \hat{\chi}_0^3 - \frac{1}{2}\beta_3 \hat{\chi}_0^4 - \frac{3}{5}\beta_4 \hat{\chi}_0^5 \right) / \beta_0 , \tag{38}$$

$$\hat{\chi}_0 = \frac{\hat{C}_0 - \hat{C}_0^A - \hat{N}_0 + \sqrt{(\hat{C}_0 - \hat{C}_0^A - \hat{N}_0)^2 + 4\hat{n}_{ie}^2}}{2n_i} , \tag{39}$$

$$\hat{C}_0^A = A_0 \hat{\chi}_0^2 \hat{C}_0 . \tag{40}$$

As can be seen from (37)-(40), Eq. (36) is a nonlinear algebraic equation relative to the unknowns $\tilde{C}_0$, $\tilde{C}_1$, and $\tilde{C}_2$. Newton's method was used for its linearization. The obtained equation linear in $\hat{C}_0$, $\hat{C}_1$, and $\hat{C}_2$ has the following form at the k+1-th iteration:

$$A_L^k \hat{C}_0^{k+1} + B_L^k \hat{C}_1^{k+1} + C_L^k \hat{C}_2^{k+1} = F_L^k , \tag{41}$$

where A_L^k, B_L^k, C_L^k, and F_L^k are the coefficients and the free term of Eq. (41), calculated with the use of the values of $\hat{C}_0^k, \hat{C}_1^k$, and $\hat{C}_2^k$ determined at the k-th iteration.

Taking into account the fact that, according to our assumptions, diffusion equation (2) is also valid at the fictitious point $i = 0$, we can write the three-point equation (32) for $i = 1$:

$$A_1^k \hat{C}_0^{k+1} + B_1^k \hat{C}_1^{k+1} + C_1^k \hat{C}_2^{k+1} = F_1^k . \tag{42}$$

From Eqs. (41) and (42) it is possible to obtain an equation for $\hat{C}_1^{k+1}$ and $\hat{C}_2^{k+1}$, eliminating the value of the impurity concentration at the left fictitious point $\hat{C}_0^{k+1}$. The resultant equation has the form

$$\hat{C}_1^{k+1} = \alpha_2^k \hat{C}_1^{k+1} + \beta_2^k , \tag{43}$$

where α_2^k and β_2^k are initial factorization coefficients. Using the obtained values of α_2^k and β_2^k, we can determine the factorization coefficients at all the nodes of the grid, including those at the right fictitious point $i = m_x + 1$.

Let us consider the factorization equation at the points $i = m_x + 1$ and $i = m_x$:

$$\hat{C}_{m_x}^{k+1} = \alpha_{m_x+1}^k \hat{C}_{m_x+1}^{k+1} + \beta_{m_x+1}^k , \tag{44}$$

$$\hat{C}_{m_x-1}^{k+1} = \alpha_{m_x}^k \hat{C}_{m_x}^{k+1} + \beta_{m_x}^k . \tag{45}$$

Now we will approximate right boundary condition (35) with second order of accuracy with respect to x. Similarly to the condition at the left boundary, we finally arrive at

$$A_R^k \hat{C}_{m_x-1}^{k+1} + B_R^k \hat{C}_{m_x}^{k+1} + C_R^k \hat{C}_{m_x+1}^{k+1} = F_R^k , \tag{46}$$

where A_R^k, B_R^k, C_R^k, and F_R^k are the coefficients and the free term of (46), calculated with the use of the values of $\hat{C}_{m_x-1}^k, \hat{C}_{m_x}^k$, and $\hat{C}_{m_x+1}^k$ at the k-th iteration.

From the system of equations (44)-(46) it is possible to evaluate $\hat{C}_{iF}^{k+1}$, i.e., the last value necessary for evaluation of the grid function C_i^{k+1} by the factorization method.

NOTATION

n_i, n_{ie}, concentration of intrinsic charge carriers and its effective value at high doping levels; D_i, intrinsic diffusion coefficient of silicon in gallium arsenide; ×, sign of the neutral charge state; $\tilde{C}_{\mathrm{Ga}_i}^{V\times}$ and $\tilde{C}_{\mathrm{AS}_i}^{V\times}$, concentrations of gallium and arsenic vacancies reduced to thermally equilibrium values in the neutral charge state; C and C^A, concentrations of atoms at the nodes of the gallium and arsenic sublattices; C^T, total concentration of silicon atoms; N, concentration of ionized atoms of a different impurity with the opposite type of conductivity; $D(\chi, T)$, effective diffusion coefficient of silicon in gallium arsenide; χ, reduced concentration of electrons; ω^2, function describing the deviation of the electron gas state from ideality at high doping levels.

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