Analytical solution of the equations describing interstitial migration of impurity atoms

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An analytical solution of the equations describing impurity diffusion due to the migration of nonequilibrium impurity interstitial atoms was obtained for the case of the Robin boundary condition on the surface of a semiconductor. The solution obtained can be useful for verification of approximate numerical solutions, for simulation of a number of processes of interstitial diffusion, and for modeling impurity diffusion in doped layers with the decanometer thickness because in these layers a disequilibrium between immobile substitutionally dissolved impurity atoms, migrating self-interstitials, and migrating interstitial impurity atoms can take place. To illustrate the latter cases, a model of nitrogen diffusion in gallium arsenide was developed and simulation of nitrogen redistribution from a doped epitaxial layer during thermal annealing of GaAs substrate was done. The calculated impurity concentration profile agrees well with experimental data. The fitting to the experimental profiles allowed us to derive the values of the parameters that describe interstitial impurity diffusion.

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I. INTRODUCTION

At present numerical methods have been widely used for simulation of solid state diffusion of ion-implanted dopants and impurity atoms added during epitaxial growth (see, for example, [1, 2, 3]). As a rule, to simulate the diffusion of impurity, a system of equations describing a coupled diffusion of different mobile species and their quasi-chemical reactions during annealing is solved. Due to a great number of differential equations and the complexity of the system as a whole, the problem of the correctness of a numerical solution is very important. One of the best ways to verify the correctness of the approximate numerical solutions is a comparison with the exact analytical solution of the boundary value problem under consideration. Such analytical solutions can be derived for the special cases of dopant or point defect diffusion. For example, in Ref. [4] an analytical solution for the point defect diffusion based on the Green function approach was obtained. It was supposed in [4] that nonequilibrium point defects were continuously generated during ion implantation of impurity atoms and diffused to the surface and into the bulk of a semiconductor. The surface was considered to be a perfect sink for point defects. In Ref. [5] a process of impurity diffusion during ion implantation at elevated temperatures was investigated analytically. It was supposed that the implantation temperature was too low to provide a traditional diffusion by the “dopant atom – point defect” pairs, but was enough for the diffusion of nonequilibrium interstitial impurity atoms to occur. Unlike [4], in Ref. [5] a system of equations, namely, the conservation law for substitutionally dissolved impurity atoms and the equation of diffusion–recombination of nonequilibrium interstitial impurity atoms have been solved analytically by the Green function approach. Reflecting boundary condition at the surface of a semiconductor has been chosen to describe the interaction of interstitial impurity atoms with the interface. Due to this condition, a diffusion problem has become symmetric with respect to the point $x = 0$. For simplicity, the condition of zero impurity concentration for $x \to \pm \infty$ has been used. It is interesting to note that analytical solutions for gold diffusion in silicon due to the Frank-Turnbull and kick-out mechanisms were obtained in Refs. [6, 7], respectively. It was supposed that there was a local equilibrium between substitutionally dissolved impurity atoms, vacancies (or self-interstitials for the kick-out mechanism) and interstitial impurity atoms. The case of nonequilibrium interstitial impurity atoms was not considered in these papers. The very interesting case of coupled diffusion of vacancies and self-interstitials was investigated in [8, 9]. The equations of the diffusion of vacancies or of self-interstitials are similar to the equation of diffusion of impurity interstitials. However, the solutions obtained in [8, 9] are difficult to use for describing the impurity diffusion governed by nonequilibrium interstitial impurity atoms, because a condition of local equilibrium was used in all these papers. Besides, a generation rate was assumed to be equal to zero in [9] or equal to a constant value in [8]. In Ref. [10] analytical one-dimensional (1D) solutions of the equations that describe impurity diffusion due to migration of nonequilibrium impurity interstitials were obtained for the case of impurity redistribution during ion implantation at elevated temperatures and for diffusion from a doped epitaxial layer. The reflecting boundary condition on the surface of a semiconductor and the conditions of constant concentration on the surface were used in the first and second cases, respectively. These analytical solutions were obtained on the finite-length 1D domain that is very convenient for comparison with numerical solution. Moreover, simulation of hydrogen diffusion in silicon during high-fluence low-energy deuterium implantation at a temperature of 250 °C and beryllium
diffusion from a doped epi-layer during rapid thermal annealing of InP/InGaAs heterostructures at a temperature of 900 °C was carried out on the basis of the analytical solutions obtained. It is interesting to note that the calculated impurity concentration profiles agree well with the experimental data that made it possible to derive the parameters of interstitial diffusion. This means that the solutions obtained are useful for solving a number of problems of solid state diffusion. The main goal of the present work is to continue the investigations of Refs. [5, 10] to obtain a similar analytical solution for a more intricate case of Robin boundary condition on the surface of a semiconductor.

II. ORIGINAL EQUATIONS

As in Refs. [5, 10], it is supposed that the processing temperature is too low to provide diffusion of substitutionally dissolved impurity atoms, but is high enough for the diffusion of impurity interstitials to occur. Nonequilibrium interstitial impurity atoms can appear due to ion implantation or due to the replacement of the impurity atom by self-interstitial from the substitutional position into the interstitial one (Watkins effect [11]), or due to dissolution of the clusters or extended defects which incorporate impurity atoms. It is also supposed that the concentration of impurity in the doped regions originating from the migration of nonequilibrium interstitials is smaller or approximately equal to the intrinsic concentration at the processing temperature. If the concentration of substitutionally dissolved dopant atoms is higher than that of impurity atoms, let us confine ourselves to the case of neutral impurity atoms in the interstitial position. Then, the system of equations describing the evolution of impurity concentration profiles includes Refs. [5, 10]:

(i) the conservation law for substitutionally dissolved impurity atoms:

$$\frac{\partial C(x,t)}{\partial t} = \frac{C^{AI}(x,t)}{\tau^{AI}} + G^{AS}(x,t),$$  \hspace{1cm} (1)

(ii) the equation of diffusion for nonequilibrium interstitial impurity atoms:

$$d^{AI}\frac{\partial^2 C^{AI}}{\partial x^2} - \frac{C^{AI}}{\tau^{AI}} + G^{AI}(x,t) = 0,$$  \hspace{1cm} (2)

or

$$-\left[\frac{\partial^2 C^{AI}}{\partial x^2} - \frac{C^{AI}}{l_{AI}^2}\right] = \frac{\tilde{g}^{AI}(x,t)}{l_{AI}^2},$$  \hspace{1cm} (3)

where

$$l_{AI} = \sqrt{d^{AI}\tau^{AI}}, \quad \tilde{g}^{AI}(x,t) = G^{AI}(x,t) \tau^{AI}.$$  \hspace{1cm} (4)

Here $C^{AI}$ is the concentration of nonequilibrium impurity interstitials; $G^{AS}$ is the rate of adding of impurity atoms, which immediately occupy the substitutional positions, or (with the negative sign) the rate of the loss of substitutionally dissolved impurity atoms due to their transfer to the interstitial position; $d^{AI}$ and $\tau^{AI}$ are the diffusivity and average lifetime of nonequilibrium interstitial impurity atoms, respectively, and $G^{AI}$ is the generation rate of interstitial impurity atoms. We use a steady-state diffusion equation for impurity interstitials, because of the relatively large average migration length of nonequilibrium interstitial impurity atoms ($l_{AI} \gg l_{fa}$, where $l_{fa}$ is the characteristic length of the decrease in the concentration of substitutionally dissolved dopant atoms) and due to the small average lifetime of nonequilibrium impurity interstitials $\tau_{AI}$ in comparison with the duration of thermal treatment $t_P$.

The system of equations (1), (2) or (1), (3) describes impurity diffusion due to migration of nonequilibrium interstitial impurity atoms. To solve this system of equations, appropriate boundary conditions are needed. Let us consider, in contrast to [5], the finite-length one-dimensional (1D) domain $[0, x_B]$, i.e., the domain used in 1D numerical modelling. The Robin boundary conditions on the surface of a semiconductor

$$w^S_1 d^{AI} \frac{\partial C^{AI}}{\partial x} \bigg|_{x=0} + w^S_2 C^{AI} \bigg|_{x=0} = w^S_3,$$  \hspace{1cm} (5)

is added to Eq. (4) in comparison with the solutions obtained in Refs. [5, 10]. A similar condition in the bulk of a semiconductor

$$w^B_1 d^{AI} \frac{\partial C^{AI}}{\partial x} \bigg|_{x=x_B} + w^B_2 C^{AI} \bigg|_{x=x_B} = w^B_3,$$  \hspace{1cm} (6)

as well as the initial conditions

$$C(x, 0) = C_0(x), \quad C^{AI}(x, 0) = C^{eq}_{AI} = const.$$  \hspace{1cm} (7)

are also used for the final formulation of the boundary value problem.

Here, $w^S_1$, $w^S_2$, $w^S_3$ and $w^B_1$, $w^B_2$, $w^B_3$ are the constant coefficients specifying the concrete type of real boundary conditions; $C^{eq}_{AI}$ is the equilibrium value of concentration of interstitial impurity atoms in the bulk of a semiconductor (it is supposed that $C^{eq}_{AI}$ is equal to zero for many cases of interstitial impurity diffusion).

To derive an analytical solution of this boundary value problem, the Green function approach [12] can be used.

III. ANALYTICAL METHOD AND SOLUTIONS

The suggestion about the immobility of substitutionally dissolved impurity atoms allows one to solve Eq. (1) independently of Eq. (2) or Eq. (3):

$$w^S_1 d^{AI} \frac{\partial C^{AI}}{\partial x} \bigg|_{x=0} + w^S_2 C^{AI} \bigg|_{x=0} = w^S_3,$$  \hspace{1cm} (5)

is added to Eq. (1), and the Robin boundary conditions on the surface of a semiconductor

$$w^B_1 d^{AI} \frac{\partial C^{AI}}{\partial x} \bigg|_{x=x_B} + w^B_2 C^{AI} \bigg|_{x=x_B} = w^B_3,$$  \hspace{1cm} (6)

as well as the initial conditions

$$C(x, 0) = C_0(x), \quad C^{AI}(x, 0) = C^{eq}_{AI} = const.$$  \hspace{1cm} (7)

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To derive an analytical solution of this boundary value problem, the Green function approach [12] can be used.
Following form:

$$C(x, t) = \frac{1}{\tau} \int_0^t C^{AI}(x, t) dt + \int_0^t G^{AS}(x, t) dt + C_0(x).$$

We will use expression (8) together with the steady-state solution of Eq. [12] obtained by the Green function approach

$$C^{AI}(x, t) = \int_0^{x_B} G(x, \xi) w(\xi, t) d\xi,$$

where the standardizing function $w(x, t)$ [12] has the following form:

$$w(\xi, t) = \frac{\tilde{g}_{AI}(\xi, t)}{l_{AI}^2} + w_S(\xi) + w_B(\xi).$$

Here $G(x, \xi)$ is the Green function for Eq. (3). Using the standardizing function $w(x, t)$ allows one to reduce the previous boundary value problem to the boundary value problem with zero boundary conditions:

$$w^S d^{AI} C^{AI} \bigg|_{x = 0} + w^2 C^{AI} \bigg|_{x = 0} = 0,$$

$$w^B d^{AI} C^{AI} \bigg|_{x = x_B} + w^2 C^{AI} \bigg|_{x = x_B} = 0.$$

The Green function for Eq. (3) with boundary conditions [11] and [12] has the following form [12]:

$$G(x, \xi) = \frac{1}{K} \begin{cases} Q_1(x)Q_2(\xi) & \text{for } 0 \leq x \leq \xi \leq x_B, \\ Q_1(\xi)Q_2(x) & \text{for } 0 \leq \xi \leq x \leq x_B. \end{cases}$$

where

$$K = Q'_1(x)Q_2(x) - Q_1(x)Q'_2(x) = \text{const}. \quad (14)$$

Here $Q_1$ and $Q_2$ are the linearly independent solutions of the homogeneous equation

$$\frac{d^2 Q}{dx^2} - \frac{Q}{l_{AI}^2} = 0$$

with the following conditions on the left boundary:

$$Q_1(0) = w^S d^{AI}, \quad Q'_1(0) = -w^S,$$

and on the right one:

$$Q_2(x_B) = w^B d^{AI}, \quad Q'_2(x_B) = -w^B.$$ 

Following [12], we can write the functions $w_S(x)$ and $w_B(x)$ as

$$w_S(x) = \begin{cases} -\frac{1}{w_1 d^{AI}} \delta(-x)w^S_3 & \text{if } w^S_1 \neq 0, \\ \frac{1}{w_2} \delta'(-x)w^S_3 & \text{if } w^S_2 \neq 0, \end{cases}$$

$$w_B(x) = \begin{cases} -\frac{1}{w_1 d^{AI}} \delta(x_B - x)w^B_3 & \text{if } w^B_1 \neq 0, \\ -\frac{1}{w_2} \delta'(x_B - x)w^B_3 & \text{if } w^B_2 \neq 0. \end{cases}$$

Let us consider the following Robin boundary condition on the surface of a semiconductor ($x = 0$):

$$-d^{AI} \frac{\partial C^{AI}}{\partial x} \bigg|_{x = 0} + v_{eff} C^{AI} \bigg|_{x = 0} = 0,$$

i.e., $w^S_1 = -1$, $w^S_2 = v_{eff}$, $w^S_3 = 0$, and, for simplicity, the Dirichlet boundary condition

$$C(x_B, t) = C^{AI}_B$$

in the bulk of the semiconductor, i.e., $w^B_1 = 0$, $w^B_2 = 1$, $w^B_3 = C^{AI}_B$. Here, $v_{eff}$ is the effective escape velocity specifying the intensity of impurity evaporation from the surface of the semiconductor.

Then, the solutions $Q_1$ and $Q_2$ have the form

$$Q_1(x) = -d^{AI} \cosh \left( \frac{x}{l_{AI}} \right) - l_{AI} v_{eff} S \sinh \left( \frac{x}{l_{AI}} \right),$$

$$Q_2(x) = -l_{AI} \sinh \left( \frac{x - x_B}{l_{AI}} \right)$$

and

$$K = -d^{AI} \cosh \left( \frac{x_B}{l_{AI}} \right) - l_{AI} v_{eff} S \sinh \left( \frac{x_B}{l_{AI}} \right) = \text{const}. \quad (24)$$
Let us consider a buried layer highly doped with impurity atoms. Such a layer can be formed by ion implantation or due to doping during epitaxy \cite{3,13,14,15}. If the impurity concentration is high, a generation of nonequilibrium interstitial impurity atoms is possible within this layer during thermal treatment. These nonequilibrium interstitial atoms can diffuse before they transfer to the substitutional position or are trapped by immobile sinks. In many cases (see, for example, impurity profiles in \cite{3,13,14,15}), the distribution of impurity atoms in an as-grown structure can be described by the Gaussian function

\[ C_0(x) = C(x, 0) = C_m \exp \left[ -\frac{(x - R_p)^2}{2\Delta R_p^2} \right] , \quad (27) \]

where \( C_m \) is the maximum value of impurity concentration; \( R_p \) is the position of the maximum, and \( \Delta R_p \) is the standard deviation.

Let us suppose that the Gaussian function can also be used to describe the spatial distribution of the generation rate of impurity interstitials:

\[ G^{AI}(x, t) = g_m^{AI} \exp \left[ -\frac{(x - R_p)^2}{2\Delta R_p^2} \right] , \quad (28) \]

where \( g_m^{AI} \) is the maximum rate of generation of interstitial impurity atoms.

Taking into consideration expressions \(26\) and \(28\) yields

\[ w(x, t) = g_m^{AI} \frac{\tau^{AI}}{T_{AI}} \exp \left[ -\frac{(x - R_p)^2}{2\Delta R_p^2} \right] - \delta'(x_B - x) C_B^{AI} . \quad (29) \]

Substituting the Green function \(25\) and the standardizing function \(29\) into expression \(9\) allows one to obtain a spatial distribution of diffusing interstitial impurity atoms:

\[ C^{AI}(x, t) = \frac{g_m^{AI}}{l_{AI}} \exp \left[ -\frac{(x - R_p)^2}{2\Delta R_p^2} \right] \int_0^x G(x, \xi) w(x, t) d\xi = \frac{g_m^{AI}}{l_{AI}} \int_0^x \left[ \frac{d'^{AI}}{l_{AI}} \cosh \left( \frac{x}{l_{AI}} \right) + l_{AI} v_{eff} S \sinh \left( \frac{x}{l_{AI}} \right) \right] \exp \left[ -\frac{(\xi - R_p)^2}{2\Delta R_p^2} \right] d\xi \]

\[ \times \left[ \sinh \left( \frac{x - \xi}{l_{AI}} \right) \right] \int_0^x \left[ \frac{d'^{AI}}{l_{AI}} \cosh \left( \frac{\xi}{l_{AI}} \right) + l_{AI} v_{eff} S \sinh \left( \frac{\xi}{l_{AI}} \right) \right] \exp \left[ -\frac{(\xi - R_p)^2}{2\Delta R_p^2} \right] d\xi \]

\[ + \frac{d'^{AI}}{l_{AI}} \cosh \left( \frac{x}{l_{AI}} \right) + l_{AI} v_{eff} S \sinh \left( \frac{x}{l_{AI}} \right) \int_0^x \sinh \left( \frac{x - \xi}{l_{AI}} \right) \exp \left[ -\frac{(\xi - R_p)^2}{2\Delta R_p^2} \right] d\xi \]

\[ + C_B^{AI} \frac{d'^{AI}}{l_{AI}} \cosh \left( \frac{x}{l_{AI}} \right) + l_{AI} v_{eff} S \sinh \left( \frac{x}{l_{AI}} \right) \int_0^x \sinh \left( \frac{\xi - x}{l_{AI}} \right) \delta'(x_B - \xi) d\xi . \quad (30) \]
Calculating the integrals on the right-hand side of expression (30), one can obtain an explicit expression for the quasistationary distribution of interstitial impurity atoms:

\[
C^{AI}(x,t) = C^{AI}_{mul} \frac{\exp(u_3)}{d^{AI} \cosh u_2^B + l_{AI} v^{S}_{eff} \sinh u_2^B} \left\{ \exp(-u_2^B) [\exp(u_3)(\text{erf} \ u_4) - \text{erf} \ u_5] + \exp(u_3)(d^{AI} + l_{AI} v^{S}_{eff}) (\text{erf} \ u_4 - \text{erf} \ u_6) \right\} + C^{AI}_{B} d^{AI} \cosh u_2^B + l_{AI} v^{S}_{eff} \sinh u_2^B,
\]

where

\[
C^{AI}_{mul} = \frac{\sqrt{\tau^{AI} \tau^{AI}} \Delta R_p}{2 \sqrt{2} l_{AI}},
\]

\[
u_1 = \frac{\Delta R_p^2 - 2l_{AI} R_p}{2l_{AI}},
\]

\[
u_2 = \frac{x}{l_{AI}},
\]

\[
u_2^B = \frac{x_B}{l_{AI}},
\]

\[
u_3 = \frac{2R_p}{l_{AI}},
\]

\[
u_4 = \frac{\Delta R_p^2 + l_{AI} R_p - l_{AI} x}{\sqrt{2} \Delta R_p l_{AI}},
\]

\[
u_4^B = \frac{\Delta R_p^2 + l_{AI} R_p - l_{AI} x_B}{\sqrt{2} \Delta R_p l_{AI}},
\]

\[
u_5 = \frac{\Delta R_p^2 - l_{AI} R_p + l_{AI} x}{\sqrt{2} \Delta R_p l_{AI}},
\]

\[
u_5^B = \frac{\Delta R_p^2 - l_{AI} R_p + l_{AI} x_B}{\sqrt{2} \Delta R_p l_{AI}},
\]

\[
u_6 = \frac{\Delta R_p^2 + l_{AI} R_p}{\sqrt{2} \Delta R_p l_{AI}},
\]

\[ u_7 = \frac{\Delta R_p^2 - l_{AI} R_p}{\sqrt{2} \Delta R_p l_{AI}}, \]

\[ u_8 = \frac{x - x_B}{l_{AI}}. \]

Postulating that the loss of substitutionally dissolved impurity atoms is equal in modulus to the rate of generation of impurity interstitials \((G^{AS}(x,t)) = -G^{AI}(x,t))\), taking into account that the distribution of impurity interstitial atoms \(C^{AI}(x,t) = C^{AI}(x)\) for the time-independent generation rate \((27)\), and substituting expressions \((27), (28), \) and \((31)\) into \((8)\), one can calculate the concentration of impurity atoms in the substitutional position

\[
C(x,t) = \frac{t}{\tau^{AI}} C^{AI}(x) + C_m (1 - p^{AI}) \exp \left( \frac{(x - R_p)^2}{2 \Delta R_p^2} \right),
\]

where \(p^{AI}\) is the fraction of the impurity atoms which transferred from the substitutional position into the interstitial one.

Expressions (31) and (44) are the obtained solution of the boundary value problem under consideration and can be used for verification of approximate numerical solutions and for simulation of interstitial diffusion.

### IV. SIMULATION

The analytical solutions (31) and (44) can be used for modeling different diffusion processes in semiconductor substrates. Below, we consider the case of nitrogen diffusion in gallium arsenide investigated in [3]. Nitrogen distributions of an as-grown and subsequently annealed specimen measured by secondary ion mass spectrometry (SIMS) are presented in Fig. 1. In [3] a GaAs layer with about 1 \(\mu\)m thickness was grown on a gallium arsenide...
Substrate at 580 °C by solid source molecular beam epitaxy. Intermediate introduction of an N$_{2}$ flow from a plasma source resulted in a buried N doping layer with a peak concentration of about 10$^7$ µm$^{-3}$ and a width of several 10 nm. This doping layer was thus sandwiched between a buffer and a cap layer of either roughly 0.5 µm thickness. Diffusion annealing was performed at a temperature of 822 °C for 15 h in sealed quartz ampoules. It can be seen from Fig. 1 that the nitrogen concentration profile after annealing is characterized by two extended low concentration “tails” directed into the bulk of the semiconductor and to its surface.

Let us consider a possible mechanism of the formation of such “tails”. In recent years the mechanism of dopant diffusion in silicon crystals due to the formation, migration, and dissociation of the “impurity atom – vacancy” or “impurity atom – self-interstitial” pairs (the pair diffusion mechanism) has become commonly accepted (see, for example [1, 16, 17, 18]). It is supposed within the framework of the pair diffusion mechanism that a local thermodynamic equilibrium prevails between substitutionally dissolved dopant atoms, intrinsic point defects, and the pairs. However, boron diffusion in silicon is often considered within the framework of the substitutional-interstitial mechanism [19, 20, 21], when the silicon self-interstitial displaces an immobile impurity atom from the substitutional to the interstitial position. A migrating interstitial impurity atom in turn replaces the host atom becoming substitutional again (the so-called “kick-out mechanism”).

It is supposed that the kick-out mechanism is also responsible for the diffusion of gold in silicon [6, 7]; zinc [22, 23, 24, 25, 26, 27, 28, 29]; nitrogen [30, 31, 32, 33]; magnesium [22, 23, 24, 25, 26, 27, 28, 29]; arsenic [34, 35, 36]; and beryllium [24, 27, 32, 35] in GaAs. As follows from the investigations presented in [27, 30, 37], beryllium diffusion in other compound semiconductors is governed by the kick-out mechanism too.

To describe diffusion due to the kick-out mechanism it is also supposed that there is a local equilibrium between substitutionally dissolved dopant atoms, self-interstitials, and interstitial dopant atoms. In this case a mathematical description of diffusion due to the kick-out mechanism is equal to the description of the pair diffusion [24]. It was shown in [22, 23, 24] within the framework of diffusion in silicon governed by the “dopant atom – self-interstitial” pairs that the formation of the extended “tail” in the low concentration region of phosphorus profile occurs if the distribution of silicon self-interstitials is nonuniform, namely, the distribution of self-interstitials in the neutral charge state have to be nonuniform [22, 23]. Thus, “tail” formation can be attributed to the nonuniform distribution of self-interstitials in the neutral charge state.

In Ref. [3] it was supposed that nitrogen diffusion in GaAs is governed by the kick-out mechanism with interstitial As as a native point defect (mathematically equivalent to the diffusion due to the “impurity atom – As self-interstitial” pairs), and that two extended low concentration “tails” on the nitrogen concentration profile are formed due to the nonuniform distribution of As interstitial atoms. In contrast to [3], it is supposed in this paper that during thermal annealing the generation of nitrogen interstitials occurs in the buried layer and that migration of these nonequilibrium interstitial atoms is responsible for the nitrogen redistribution. In our opinion, this mechanism of diffusion is more preferable because the atomic radius of nitrogen is smaller than arsenic radius and hence in the doped GaAs the nonequilibrium nitrogen interstitials prevail rather than the arsenic ones. In addition, it was shown in [40] that the mass action law and local thermodynamic equilibrium between substitutionally dissolved dopant atoms, vacancies, and vacancy-impurity pairs are not valid in the low concentration regions of the abrupt dopant profile formed by low energy ion implantation. This conclusion is also true for diffusion due to the “dopant atom – self-interstitial” pairs and due to the kick-out mechanism. It is important to note that the buried nitrogen layer investigated in [3] is very narrow and disequilibrium between substitutionally dissolved impurity atoms and diffusing species may well occur. Therefore, we try to explain the experimental data of [3] within the framework of migration of nonequilibrium nitrogen interstitials.

In Fig. 1 the results of simulation of nitrogen diffusion in GaAs obtained on the basis of analytical solution (31) and (44) are presented.

![Graph](image-url)

**Fig. 1:** Calculated nitrogen concentration profile (solid line) after thermal treatment of a GaAs substrate containing a buried nitrogen layer with a width of several 10 nm at a temperature of 822 °C for 15 h. The experimental data (dots) are taken from Stolwijk et al. [3].

The following values of simulation parameters were used to fit the calculated curve to the experimental nitrogen profile: i) the parameters of the as-grown nitrogen distribution: $C_m = 0.66 \times 10^7$ µm$^{-3}$; $R_P = 0.468$ µm; $\Delta R_P = 0.016$ µm; ii) the parameters of the nitrogen interstitial diffusion: $T^{AI} = 0.16$ µm; $\tau^{AI} = 0.1$ s; $g_m^{AI} = 102.0$ µm$^{-3}$s$^{-1}$; $g^{AI} = 0.84$; $v_{eff} = 1.5$ µm s$^{-1}$.

As can be seen from Fig. 1 the calculated curve agrees well with the measured nitrogen concentration profile. Thus, the experimental data [3] can be explained on the basis of the migration of nonequilibrium nitrogen interstitials. It follows from the value of the fitting parameter
that approximately 84% of the nitrogen atoms from the buried layer are being transferred to the transient interstitial positions. Migration of these nonequilibrium interstitial atoms results in the formation of two extended “tails” on the nitrogen concentration profile.

V. CONCLUSIONS

The analytical solution of the equations that describe impurity diffusion due to migration of nonequilibrium impurity interstitials is obtained for the case of Robin boundary condition on the surface of a semiconductor. Using this solution, one can verify the correctness of the approximate numerical calculations obtained by the codes intended for simulation of diffusion processes. Moreover, it is possible to carry out an analytical simulation of a number of diffusion processes which are based on the migration of impurity interstitial atoms and can be used in the fabrication of semiconductor devices. The solution obtained can also be useful for simulation of impurity diffusion in the doped layers with decanometer thickness because in these layers disequilibrium between immobile substitutionally dissolved impurity atoms, migrating self-interstitials, and migrating interstitial impurity atoms can take place. As an example, nitrogen redistribution from a buried layer during thermal annealing of GaAs substrate at a temperature of 822 °C for 15 h have been simulated. By comparison with the experimental data, the values of the parameters that describe interstitial nitrogen migration have been derived. For example, it was found that for the process under consideration approximately 84% of the nitrogen atoms occupied transient interstitial positions and the average migration length of these interstitial impurity atoms was 0.16 μm.

[1] T. Uchida, K. Eikyu, E. Tsuchida, M. Fujinaga, A. Teramotio, T. Yamashita, T. Kunikiyio, K. Ishikawao, N. Katori, S. Kawazau, C. Hamaguchi, T. Nishimura, Simulation of dopant redistribution during gate oxidation including transient-enhanced diffusion caused by implantation damage, *Jpn. J. Appl. Phys. Pt.1*, **39**, No.5A, 2565-2576 (2000).

[2] F. Boucard, F. Roger, I. Chakarovo, V. Zhuk, M. Temkin, X. Montagner, E. Guichard, D. Mathiot, A comprehensive solution for simulating ultra-shallow junctions: From high dose/low energy implant to diffusion annealing, *Mat. Sci. Eng. B*, **124-125**, 409-414 (2005).

[3] N. A. Stolwijk, G. Bösker, T. G. Andersson, U. Södervall, Diffusion of nitrogen in gallium arsenide, *Physica B*, **340-342**, 367-370 (2003).

[4] R. L. Minear, D. C. Nelson, J. F. Gibbons, Enhanced diffusion in Si and Ge by light ion implantation, *J. Appl. Phys.*, **43**, No.8, 3468-3480 (1972).

[5] O. I. Velichko, Atomic diffusion processes in a nonequilibrium state of the components in a defect-impurity system of silicon crystals, Dissertation, Minsk, Institute of Electronics of the National Academy of Sciences of Belarus, 1988 (in Russian).

[6] U. Gosele, W. Frank, A. Seeger, Mechanism and kinetics of the diffusion of gold in silicon, *Appl. Phys.*, **23**, 361–368 (1980).

[7] A. Seeger, On the theory of the diffusion of gold into silicon, *Phys. Stat. Sol. A*, **61**, 521–529 (1980).

[8] T. Hashimoto, Steady-state solution of point-defect diffusion profiles under irradiation, *Jpn. J. Appl. Phys.*, **29**, No.1, 177–178 (1990).

[9] T. Okino, T. Shimoseki, R. Takae, M. Onishi, Steady state solutions of diffusion equations of self-interstitials and vacancies in silicon, *Jpn. J. Appl. Phys. Pt.1*, **34**, No.12A, 6298–6302 (1995).

[10] O. I. Velichko and N. A. Sobolevskaya, Analytical solutions for the interstitial diffusion of impurity atoms, *Nonlinear Phenomena in Complex Systems*, **10**, No.4, 376–384 (2007).

[11] G. D. Watkins, A microscopic view of radiation damage in semiconductors using EPR as a probe, *IEEE Trans., NS-16*, No.6, 13–18 (1969).

[12] A. G. Butkovskiy, *Harakteristiksi sistem s raspredelennymi parametrami (Characteristics of Distributed-Parameter Systems)*, Nauka, Moscow, 1979 (in Russian).

[13] D. J. Eaglesham, P. A. Stolk, H.-J. Gossmann, J. M. Poate, Implantation and transient B diffusion in Si: The source of the interstitials, *Appl. Phys. Lett.*, **65**, No.18, 2305–2307 (1994).

[14] D. Skarlatos, D. Tsoukalas, L. F. Giles, A. Claverie, Point defect injection during nitrous oxidation of silicon at low temperatures, *J. Appl. Phys.*, **87**, No.3, 1103–1109 (2000).

[15] S. Mirabella, A. Coati, S. Scalese, D. De Salvador, S. Pulvirenti, G. Bisognin, E. Napolitani, A. Terrasi, M. Berti, A. Carnera, A. V. Drigo, F. Priolo, Suppression of boron transient enhanced diffusion by C trapping, *Solid State Phenomena*, **82–84**, 195–200 (2002).

[16] O. I. Velichko, "A set of equations of radiation-enhanced diffusion of ion-implanted impurities", in: I. I. Danilovich, A. G. Koval’, V. A. Labunov et al. (Eds.), Proceedings of VII International Conference "Vzaimodeystvie Atomnyh Chastits s Tverdym T elom (Interaction of Atomic Particles with Solid)", Part 2, Minsk, Belarus, 180-181 (1984) (in Russian).

[17] D. Mathiot, S. Martin, Modeling of dopant diffusion in silicon: An effective diffusivity approach including point-defect couplings, *J. Appl. Phys.*, **70**, No.6, 3071–3080 (1991).

[18] *TSUPREM—4 User’s Manual. Version 2000.4*. Avant! Corp. (Fremont. CA. December 2000).

[19] M. Uematsu, Simulation of boron, phosphorus, and arsenic diffusion in silicon based on an integrated diffusion model, and the anomalous phosphorus diffusion mechanism, *J. Appl. Phys.*, **82**, No.5, 2228–2246 (1997).

[20] L. Iach’adene-Le Coq, J. Marcon, A. Dush-Nicolini, K. Masmoudi, K. Ketata, Diffusion simulations of boron implanted at low energy (500 eV) in crystalline silicon, *Nuclear Instrum. Meth. Phys. Res. B*, **216**, 303–307 (2004).

[21] I. Martin-Bragado, R. Pinacho, P. Castrillo, M. Jaraiz, J.
E. Rubio, J. Barbolla, Physical modeling of Fermi-level effects for decananano device process simulations, *Mat. Sci. Eng. B*, **114–115**, 284–289 (2004).

[22] U. Gösele and F. Morehead, Diffusion of zinc in gallium arsenide: A new model, *J. Appl. Phys.*, **52**, No.7, 4617–4619 (1981).

[23] S. Reynolds, D. W. Vook, J. F. Gibbons, Open-tube Zn diffusion in GaAs using diethylzinc and trimethylarsenic: Experiment and model, *J. Appl. Phys.*, **63**, No.4, 1052–1059 (1988).

[24] S. Yu, T. Y. Tan, U. Gösele, Diffusion mechanism of zinc and beryllium in gallium arsenide, *J. Appl. Phys.*, **69**, No.6, 3547–3565 (1991).

[25] G. Bösker, N. A. Stolwijk, H.-G. Hettwer, A. Rucki, W. Jäger, U. Södervall, Use of zinc diffusion into GaAs for determining properties of gallium interstitials, *Phys. Rev. B*, **52**, No.16, 11927–11931 (1995).

[26] M. P. Chase, M. D. Deal, J. D. Plummer, Diffusion modeling of zinc implanted into GaAs, *J. Appl. Phys.*, **81**, No.4, 1670–1676 (1997).

[27] C.-H. Chen, U. M. Gosele, T. Y. Tan, Dopant diffusion and segregation in semiconductor heterostructures: Part 1. Zn and Be in III-V compound superlattices, *Appl. Phys. A*, **68**, 9–18 (1999).

[28] H. Bracht, M. S. Norseng, E. E. Haller, K. Eberl, Zinc diffusion enhanced Ga diffusion in GaAs isotope heterostructures, *Physica B*, **308–310**, 831–834 (2001).

[29] H. Bracht, S. Broitzmann, Zinc diffusion in gallium arsenide and the properties of gallium interstitials, *Phys. Rev. B*, **71**, 115216 (10 pp.) (2005).

[30] G. Bösker, N. A. Stolwijk, J. V. Thordson, U. Södervall, and T. G. Andersson, Diffusion of nitrogen from a buried doping layer in gallium arsenide revealing the prominent role of As interstitials, *Phys. Rev. Let.*, **81**, No.16, 3443–3446 (1998).

[31] N. A. Stolwijk, G. Bösker, J. V. Thordson, U. Södervall, T. G. Andersson, Ch. Jäger, W. Jäger, Self-diffusion on the arsenic sublattice in GaAs investigated by the broadening of buried nitrogen doping layers, *Physica B*, **273-274**, 685–688 (1999).

[32] H.G. Robinson, M.D. Deal, D.A. Stevenson, Damage-induced uphill diffusion of implanted Mg and Be in GaAs, *Appl. Phys. Lett.*, **56**, No.6, 554–556 (1990).

[33] H. G. Robinson, M. D. Deal, D A. Stevenson, Hole-dependent diffusion of implanted Mg in GaAs, *Appl. Phys. Lett.*, **58**, No.24, 2800–2802 (1991).

[34] H. D. Robinson, M. D. Deal, G. Amaratunga, P. B. Griffin, D. A. Stevenson, J. D. Plummer, Modeling uphill diffusion of Mg implants in GaAs using SUPREM - IV, *J. Appl. Phys.*, **71**, No.6, 2615–2623 (1992).

[35] J. C. Hu, M. D. Deal, J. D. Plummer, Modeling the diffusion of grown-in Be in molecular beam epitaxy GaAs, *J. Appl. Phys.*, **78**, No.3, 1595-1605 (1995).

[36] K. Ketata, M. Ketata, S. Kountz, J. Marcon, O. Valet. Modeling the diffusion of Be in InGaAs/InGaAsP epitaxial heterostructures under non-equilibrium point defect conditions, *Physica B*, **273-274**, 823–826 (1999).

[37] M. Ihaddadene-Lenglet, J. Marcon. Optimization of InGaAs/InP MHB and HBT’s technology: control and modeling of beryllium diffusion phenomena, *Nucl. Instrum. Meth. Phys. Res. B*, **216**, 297–302 (2004).

[38] O. I. Velichko, Mechanism of the locally enhanced impurity diffusion under high concentration doping of silicon with phosphorus, *Elektronnaya tehnika. Ser. 2. Poluprovodnikovye pribory* (Electronic Technics. Part 2. Semiconductor Devices), Issue 2(187), 57–63 (1987) (in Russian).

[39] M. Orlowski, Unified model for impurity diffusion in silicon, *Appl. Phys. Lett.*, **53**, No.14, 1323–1326 (1988).

[40] O. I. Velichko, Local thermodynamic disequilibrium during rapid thermal annealing of ion-implanted silicon, *Radiotekhnika i Elektronika, Republican interdepartmental volume of papers, Minsk, Belarus*, Issue 15, 106-110 (1986) (in Russian).