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Solutions of diffusion equation for point defects

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Abstract. An analytical solution of the equation describing diffusion of intrinsic point defects in semiconductor crystals has been obtained for a one-dimensional finite-length domain with the Robin-type boundary conditions. The distributions of point defects for different migration lengths of defects have been calculated. The exact analytical solution was used to verify the approximate numerical solution of diffusion equations for vacancies and self-interstitials. Based on the numerical solution obtained, investigation of the diffusion of silicon self-interstitials in a highly doped surface region formed by ion implantation was carried out.

Keywords: silicon, implantation, point defect diffusion, modeling.
AMS Subject Classification: 81T80, 97M50, 34B27.

1 Introduction

The electrophysical parameters of silicon integrated microcircuits and other semiconductor devices are determined by the state of a defect-impurity system of doped regions. Now, submicron regions of semiconductor devices are formed by means of ions implantation with subsequent low-budget thermal annealing. During annealing, the main fraction of the nonequilibrium defects generated by ion implantation is eliminated. As hydrogen atoms readily passivate dangling bonds, introduction of hydrogen into silicon substrates can be used for further improvements in the device performance by

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decreasing the imperfections of the crystalline lattice and eliminating undesirable electronic states from the band gap [12]. Introduction of hydrogen can be carried out by means of silicon treatment in a hydrogen-containing plasma [12,35] or due to implantation of hydrogen ions. In both cases introduction of hydrogen ions is accompanied by generation of additional defects in the near surface region. Due to the smallness of hydrogen atoms, it is found that single point defects, namely, vacancies and self-interstitials, will be generated in undoped silicon. On the other hand, after implantation of a high fluence of hydrogen ions, due to the diffusion and quasichemical reactions of generated point defects among themselves, with hydrogen atoms and other imperfections of the crystalline lattice, a thin heavily damaged layer, i. e., a quite deep weakened zone can be formed in the bulk of a semiconductor. As a result, the active layer with SiO_2 isolation can be separated from the rest of the bulk substrate due to the splitting that takes place inside the weakened zone. This is the way in which different structures called silicon-on-insulator (SOI) are formed [7] which have a number of advantages in comparison with the electric isolation fabricated by the traditional technology.

It is worth noting that nonequilibrium point defects can be mobile even at room temperature. Indeed, according to the temperature dependence obtained in the paper [22], the diffusivity of silicon self-interstitials atoms $d_i^I = 1.06\ \mu\mathrm{m}^2/\mathrm{s}$ for a temperature of 300 K. On the other hand, it follows from the data of [11] that this diffusivity is equal to $3.2{\times}10^4 \mu\mathrm{m}^2/\mathrm{s}$. The characteristic diffusion length of silicon self-interstitials $L^I = \sqrt{d_i^I t}$ obtained for these values of diffusivity varies from 3.26 μm to 566 μm for the time duration $t = 10$ s. It means that even at room temperature silicon self-interstitials diffuse easily far away from the boundaries of the active regions. Thus, distributions of nonequilibrium point defects in fabricated semiconductor devices are determined not only by their generation in the local domains, but also by the diffusion-induced defect redistribution.

To calculate the distributions of point defects, Minear et al. [19] obtained an analytical solution of the equation

$$d_i \frac{d^2 C^D}{d\,x^2} - \frac{C^D}{\tau_i} + G^R(x) = 0 \tag{1}$$

that describes diffusion of point defects in the semiinfinite interval $[0,+\infty]$. The case of constant coefficients d_i and τ_i was considered. Here $C^D = C^D(x)$ is the concentration of point defects; d_i and τ_i are the diffusivity and average lifetime of point defects in an intrinsic semiconductor, respectively.

It was supposed in [19] that nonequilibrium point defects were contin-

uously 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. The concentration of nonequilibrium defects was also set equal to zero at infinity. It was supposed that the generation of nonequilibrium point defects is determined by two factors, namely, the generation due to the primary Rutherford scattering and secondary cascades and the generation by hard-sphere interaction at or near the end of the ion's track. Then, the total generation rate of point defects in the volume unit can be approximated by an expression with two summands:

$$G^{R} = G_{m}^{Ru} \operatorname{erfc}\left(\frac{x - R_{p}}{\Delta R_{p}}\right) + G_{m}^{R} \exp\left[-\frac{(x - R_{p})^{2}}{2\Delta R_{p}^{2}}\right] , \qquad (2)$$

where G_{m}^{Ru} and G_{m}^{R} are the maximal values of point defect generation rates for the processes described above; R_p and ΔR_p are the average projective range of implanted ions and straggling of the projective range, respectively.

A similar solution was obtained in [27] for the Robin boundary condition on the surface of a semiconductor:

$$- d_{i} \left.\frac{d C^{D}}{d x}\right|_{x=0} + \mathrm{v}^{S} C^{D}(0) = 0 \ , \qquad (3)$$

where v^{S} is the parameter describing the velocity of point defect trapping on the surface of a semiconductor. Only the second term in the right-hand side of expression (2) is used for the generation rate of nonequilibrium defects.

At present, in the modern silicon technology, different layered structures such as $\mathrm{Si_{1-x}Ge_x/Si}$ [3, 15, 26] and silicon-on-insulator [7] are widely used. Therefore, it is reasonable to obtain an analytical solution of the equation for diffusion of intrinsic point defects in a finite-length domain $[0, x_B]$. The solution obtained can be helpful for studying the form of point defect distributions under characteristic conditions used in processing semiconductor substrates and for verification of numerical solutions. This solution can be also applied for modeling a number of the processes of diffusion of vacancies and silicon self-interstitials because the parameters describing the transport processes of point defects in silicon and known from the literature differ by many orders of magnitude [24].

2 The boundary-value problem on defect diffusion

The diffusion equations for vacancies and silicon self-interstitials that take into account different charge states of intrinsic point defects and drift of the charged species in the built-in electric field were obtained in [29,30]. In one-dimensional domain these equations have the following form:

1) equation of vacancy diffusion

$$\begin{aligned} \frac{\partial}{\partial x}\left[d^{V}(\chi)\,\frac{\partial \tilde{C}^{V\times}}{\partial x}\right] - \frac{\partial}{\partial x}\left[(\omega^{\chi}-1)\,\frac{\partial\, d^{V}(\chi)}{\partial \xi}\frac{\partial \xi}{\partial x}\,\tilde{C}^{V\times}\right] \\ + \frac{S^{E}-G^{E}}{C^{V\times}_{eq}} - k^{AIkV}(\chi)\; C^{AIk}\;\tilde{C}^{V\times} \\ - k^{IV}(\chi)\; C^{I\times}_{eq}\;\tilde{C}^{I\times}\;\tilde{C}^{V\times} - \frac{S^{V}}{C^{V\times}_{eq}} \\ + \frac{G^{VT}+G^{VR}}{C^{V\times}_{eq}} = 0. \end{aligned} \tag{4}$$

2) equation for diffusion of silicon self-interstitial

$$\begin{aligned} \frac{\partial}{\partial x}\left[d^{I}(\chi)\,\frac{\partial \tilde{C}^{I\times}}{\partial x}\right] - \frac{\partial}{\partial x}\left[(\omega^{\chi}-1)\,\frac{\partial\, d^{I}(\chi)}{\partial \xi}\frac{\partial \xi}{\partial x}\,\tilde{C}^{I\times}\right] \\ + \frac{S^{F}-G^{F}}{C^{I\times}_{eq}} - k^{W}(\chi)\;\tilde{C}^{I\times} \\ + \frac{k^{AIk}}{C^{I\times}_{eq}}C^{AIk} - k^{IV}(\chi)\; C^{V\times}_{eq}\;\tilde{C}^{V\times}\;\tilde{C}^{I\times} \\ - \frac{S^{I}}{C^{I\times}_{eq}} + \frac{G^{IT}+G^{IR}}{C^{I\times}_{eq}} = 0, \end{aligned} \tag{5}$$

where

$$\chi = \frac{\xi + \sqrt{\xi^{2}+4n_i^{2}}}{2n_i}\,, \tag{6}$$

$$\omega^{\chi} = \frac{\chi}{k_B T}\frac{\partial\,\mu^{\chi}}{\partial\,\chi}\,, \tag{7}$$

$$\xi = C - C^B. \tag{8}$$

Here $\tilde{C}^{V\times}$ and $\tilde{C}^{I\times}$ are respectively the concentrations of nonequilibrium vacancies and silicon self-interstitials in the neutral charge state, normalized to the equilibrium concentrations of these species $C_{eq}^{V\times}$ and $C_{eq}^{I\times}$; C and C^B are the concentrations of substitutionally dissolved impurity and impurity with the opposite type of conductivity, respectively; C^{AIk} is the concentration of impurity interstitials in a charge state k; χ is the concentration of charge carriers (electrons n or holes p for doping with donor or acceptor impurities, respectively) normalized to the intrinsic concentration of charge carriers n_i; ω^χ is the function which describes a deviation of an electron (hole) system beyond the perfect solubility; μ^χ is the chemical potential of electrons (holes); $d^V(\chi)$ is the effective diffusivity of vacancies; k^{AIkV} and k^{IV} are respectively the effective recombination coefficients of impurity interstitials (in a charge state k) and silicon self-interstitials with vacancies; G^E and S^E are the rates of generation and dissolution of the "impurity atom – vacancy" pairs; S^V is the rate of trapping the vacancies on the immobile imperfections of a crystalline lattice; G^{VT} and G^{VR} are the rates of thermal generation of vacancies and generation of vacancies due to external irradiation; $d^I(\chi)$ is the effective diffusivity of silicon self-interstitials; k^W is the effective coefficient of the replacement of the impurity atom by self-interstitial from the substitutional position into the interstitial one (Watkins effect [32]); k^{AIk} is the effective coefficient of displacement of impurity atoms from an interstitial to the substitutional position (phenomenon opposite to the Watkins effect); G^F and S^F are the rates of generation and dissolution of the "impurity atom – silicon self-interstitial" pairs; S^I is the rate of trapping the silicon self-interstitials on the immobile sinks of a crystalline lattice; G^{IT} and G^{IR} are the rates of the thermal generation of silicon self-interstitials and their generation due to external irradiation.

The diffusion equations obtained have the following characteristic features:

(i) these two equations describe diffusion of all point defects with different charge states as a whole, although only the concentration of the neutral vacancies $\tilde{C}^{V\times}$ and silicon self-interstitials $\tilde{C}^{I\times}$ must be derived to solve equations (4) and (5), respectively. After the solution, the distributions of charged species, namely, vacancies in a charge state r and silicon self-interstitials in a charge state q, can be calculated from the expressions describing the local thermodynamic equilibrium $C^{Vr} = \tilde{C}^{V\times} C_{eq}^{V\times} h^{Vr} \chi^{-zz^{Vr}}$

and $C^{Iq} = \tilde{C}^{I\times} C^{I\times}_{eq} h^{Iq} \chi^{-z z^{Iq}}$. Here z, z^{Vr}, and z^{Ir} are respectively the charge of a substitutional impurity atom, the charge of a vacancy in the charge state r, and the charge of a silicon self-interstitial in the charge state q in terms of the elementary charge; h^{Vr} and h^{Iq} are the constants of the mass action law for reactions of defects conversion from neutral to nonzero charge states;

(ii) the equations obtained take into account the drift of all charged species due to the built-in electric field. At the same time, there is no explicit term that would describe the drift and be proportional to the first derivative of the concentration of mobile species that substantially complicates the numerical solution. To exclude this term, a system of equations describing the diffusion of intrinsic point defects in each charge state was written. Then, the special mathematical transformations of these equations were performed using the mass action law for conversions between different charge states of vacancies and self-interstitials. As a result of these transformations, the drift of vacancies and silicon self-interstitials in the electric field are taken into account in the effective diffusion coefficients $d^V(\chi)$ and $d^I(\chi)$;

(iii) the effective diffusion coefficients $d^V(\chi)$ and $d^I(\chi)$ as well as the effective coefficients of quasichemical reactions $k^W(\chi)$, $k^{AIkV}(\chi)$, and $k^{IV}(\chi)$ are smooth and monotone functions of the concentration of dopant atoms.

3 Simplification of the generalized equations describing the diffusion of intrinsic point defects

The obtained generalized equations of point defect diffusion allow us to construct a family of more simple equations depending on different assumptions used for simplification. The simplified equations obtained will keep the basic features of the original equations that provide a wide region of their application. For example, the characteristic temperatures of modern semiconductor substrate treatments are within the range of hundreds Celsius degrees and often exceed 1000 °C. At such temperatures, the state of the electron (hole) gas is close to ideal even for high doping levels. It means that the function $\omega^\chi \approx 1$ for all doping levels of a semiconductor. Due to the assumption that $\omega^\chi \approx 1$, the equations of point defect diffusion are significantly simplified and can be written for a one-dimensional (1D) domain in the following form:

$$\frac{d}{d\,x}\left[d^{V}\left(\chi\right)\,\frac{d\,\tilde{C}^{V\times}}{d\,x}\right]-\frac{G^{E}-S^{E}}{C_{eq}^{V\times}}-k^{IV}\left(\chi\right)\,C_{eq}^{I\times}\,\tilde{C}^{I\times}\,\tilde{C}^{V\times}$$
$$-\frac{S^{V}}{C_{eq}^{V\times}}+\frac{G^{VT}+G^{VR}}{C_{eq}^{V\times}}=0, \tag{9}$$

$$\frac{d}{d\,x}\left[d^{I}\left(\chi\right)\,\frac{d\,\tilde{C}^{I\times}}{d\,x}\right]-\frac{G^{F}-S^{E}}{C_{eq}^{I\times}}-k^{IV}\left(\chi\right)\,C_{eq}^{V\times}\,\tilde{C}^{V\times}\,\tilde{C}^{I\times}$$
$$-\frac{S^{I}}{C_{eq}^{I\times}}+\frac{G^{IT}+G^{IR}}{C_{eq}^{I\times}}=0. \tag{10}$$

Note that the ordinary derivative on the coordinate x is used in the equations obtained for the convenience of analytical solution. It is possible because the diffusion equations are quasistationary. Indeed, the time dependence of point defect concentration is governed by the change in the distribution of impurity atoms that diffuse significantly slowly in comparison with the vacancies and silicon self-interstitials.

Let us consider the following assumption. If the diffusion of impurity atoms is negligible, the terms of equation describing the generation (absorption) of intrinsic point defects due to the dissolution (formation) of "impurity atom – intrinsic point defect" pairs are equal to zero. In this case, Eqs. (9) and (10) are reduced to the form

$$\frac{d}{d\,x}\left[d^{V}\left(\chi\right)\,\frac{d\,\tilde{C}^{V\times}}{d\,x}\right]-k^{IV}\left(\chi\right)\,C_{eq}^{I\times}\,\tilde{C}^{I\times}\,\tilde{C}^{V\times}-\frac{S^{V}}{C_{eq}^{V\times}}+\frac{G^{VT}+G^{VR}}{C_{eq}^{V\times}}=0, \tag{11}$$

$$\frac{d}{d\,x}\left[d^{I}\left(\chi\right)\,\frac{d\,\tilde{C}^{I\times}}{d\,x}\right]-k^{IV}\left(\chi\right)\,C_{eq}^{V\times}\,\tilde{C}^{V\times}\,\tilde{C}^{I\times}-\frac{S^{I}}{C_{eq}^{I\times}}+\frac{G^{IT}+G^{IR}}{C_{eq}^{I\times}}=0. \tag{12}$$

If the terms describing the absorption of point defects in Eqs. (11) and (12) are expressed as one term, we obtain the following two equations:

$$\frac{d}{d\,x}\left[d_{i}^{V}\,d^{VC}\left(\chi\right)\,\frac{d\,\tilde{C}^{V\times}}{d\,x}\right]-k_{i}^{V}\,k^{VC}\left(\chi\right)\,\tilde{C}^{V\times}+\frac{G^{VT}+G^{VR}}{C_{eq}^{V\times}}=0, \tag{13}$$

$$\frac{d}{d\,x}\left[d_i^I d^{IC}\left(\chi\right)\,\frac{d\,\tilde{C}^{I\times}}{d\,x}\right]-k_i^I k^{IC}\left(\chi\right)\,\tilde{C}^{I\times}+\frac{G^{IT}+G^{IR}}{C_{eq}^{I\times}}=0. \tag{14}$$

Here d_i^V and d_i^I are respectively the diffusivities of vacancies and self-interstitials in intrinsic silicon; $k_i^V=1/\tau_i^V$, and $k_i^I=1/\tau_i^I$ are respectively the absorption coefficients of vacancies and of silicon self-interstitials in an intrinsic semiconductor; $d^{VC}(\chi)$, $d^{IC}(\chi)$, $k^{VC}(\chi)$ and $k^{IC}(\chi)$ are the normalized dependences of corresponding quantities on the concentration of impurity atoms.

It is to be noted that Eqs. (13) and (14) are very convenient for numerical solution and studying the fundamentals of diffusion processes owing to the features (i), (ii), and (iii). In addition, it follows from these equations that for defect diffusion in an intrinsic or homogeneously doped semiconductor all nonlinear coefficients are converted into constants. Then, Eqs. (13) and (14) can be presented in the form

$$d_i\,\frac{d^2\,\tilde{C}^{\times}}{d\,x^2}-\frac{\tilde{C}^{\times}}{\tau}+\frac{G^T+G^R}{C_{eq}^{\times}}=0, \tag{15}$$

where τ is the average lifetime of point defects and d_i is the diffusivity of point defects in intrinsic silicon (we do not concretize the defect species). It is worth noting that τ is not a constant in the case of strong recombination of silicon self-interstitials with vacancies.

The equations of diffusion of the point defects, which are similar to Eqs. (13) and (14), are used in [4, 13, 18] together with the equation of impurity diffusion in modeling of the redistribution of impurity atoms in silicon. Note that the nonstationary equations of point defect diffusion are presented in the papers mentioned above. Furthermore, in contrast to Eqs. (13) and (14), the generation of intrinsic point defects due to the external influence is not considered. We shall note that due to the significant mobility of vacancies and silicon self-interstitials in comparison with impurity atoms it is reasonable to use the stationary diffusion equation for point defects, except for the cases of spike annealing [1, 9, 10, 14, 16, 21, 23, 33] and millisecond annealing [9, 10, 14, 16, 20, 21, 23] characterized by very short duration.

In a number of cases concerned with the impurity and point defect diffusion, it is possible to neglect the mutual interactions of vacancies and interstitial atoms. For example, under low-temperature oxidation of the surface of a semiconductor, silicon self-interstitials are the dominating defects in a

silicon crystal [2]. Therefore, one can neglect calculation of vacancy distribution in modeling the processes of impurity diffusion due to the negligible vacancy concentration. In this case, the average lifetime of other defects (silicon self-interstitials) can be assumed to be constant $\tau = \tau_i = const$. Here τ_i is the average lifetime of defects in an intrinsic semiconductor under equilibrium conditions. Using the quantity of the average migration length of point defects $l_i = \sqrt{d_i \tau_i}$, one can present the equation of diffusion (15) in the following form:

$$\frac{d^2 \tilde{C}^{\times}}{d x^2} - \frac{1}{l_i^2} \tilde{C}^{\times} + \frac{1 + \tilde{g}\,(x,t)}{l_i^2} = 0, \tag{16}$$

where $\tilde{g}\,(x,t) = G^R/G^T$ represents the generation rate of point defects under consideration in the volume unit of a semiconductor normalized to the thermal generation rate of these defects.

Let us obtain a solution of Eq. (16) in the 1D finite-length domain $[0, x_B]$ for $\tilde{g}\,(x,t) = \tilde{g}\,(x)$ and the Robin boundary conditions on the left and right boundaries:

$$- w_1^S d_i \frac{d\,\tilde{C}^{\times}}{d\,x}\bigg|_{x\,=\,0} + w_2^S \tilde{C}^{\times}(0) = w_3^S, \tag{17}$$

$$- w_1^B d_i \frac{d\,\tilde{C}^{\times}}{d\,x}\bigg|_{x\,=\,x_B} + w_2^B \tilde{C}^{\times}(x_B) = w_3^B, \tag{18}$$

where w_1^S, w_2^S, w_3^S, w_1^B, w_2^B, and w_3^B are the constant coefficients specifying the concrete type of real boundary conditions.

4 Analytical solution of the equation describing defect diffusion

For the solution of the boundary-value problem (16), (17), and (18) we can use the Green function approach [6]:

$$\tilde{C}^{\times}(x,t) = \int_0^{x_B} G(x,\xi)\,\omega\,(\xi)\,d\xi, \tag{19}$$

where the standardizing function $\omega(\xi)$ has the following form:

$$\omega(\xi) = \frac{1 + \tilde{g}\,(x,t)}{l_i^2} + \omega_S(\xi) + \omega_B(\xi), \tag{20}$$

and $G(x,\xi)$ is the Green's function for Eq. (16). Using the standardizing function $\omega(\xi)$ [6] allows one to reduce the previous boundary-value problem to the boundary-value problem with boundary conditions having zero right-hand sides:

$$- w_1^S d_i \frac{d\tilde{C}^{\times}}{dx}\bigg|_{x\,=\,0} + w_2^S \tilde{C}^{\times}(0) = 0, \qquad (21)$$

$$- w_1^B d_i \frac{d\tilde{C}^{\times}}{dx}\bigg|_{x\,=\,x_B} + w_2^B \tilde{C}^{\times}(x_B) = 0. \qquad (22)$$

Let us consider the following Robin boundary condition on the left boundary of the layer (for example, on the surface $x = 0$) and in the bulk of a semiconductor $x = x_B$:

$$w_1^S = 1, \qquad w_2^S \neq 0, \qquad w_3^S = 0, \qquad (23)$$

$$w_1^B = 1, \qquad w_2^B \neq 0, \qquad w_3^B = 0. \qquad (24)$$

These boundary conditions are very interesting for technology because they allow one to describe the flux of point defects through the left and the right boundaries as well as the absorption of defects on the boundary [27]. Then, it follows from [6] that $\omega_S(x) = 0$ and $\omega_B(x) = 0$.

Let us assume that the generation of nonequilibrium point defects occurs due to the ion implantation and that the distribution of their generation rate is approximated by the Gaussian function:

$$\tilde{g}\,(x,t) = g_m \exp\left[-\frac{(x - R_{pd})^2}{2\Delta R_{pd}^2}\right], \qquad (25)$$

where g_m is the maximum rate of generation of nonequilibrium defects normalized to the rate of the thermal generation of this species; R_{pd} is the position of the generation maximum and ΔR_{pd} is the standard deviation.

Substituting the Green function [6] and expression (25) into (19) allows one to obtain the spatial distribution of point defect concentration:

$$\tilde{C}^{\times}(x) = \tilde{C}^{\times}_{eq}(x) + \tilde{C}^{\times}_{R}(x), \qquad (26)$$

where $\tilde{C}^{\times}_{eq}(x)$ is the distribution of point defect concentration in the case of zero external radiation and $\tilde{C}^{\times}_{R}(x)$ is the change of defect concentration

due to the ion implantation:

$$\tilde{C}^{\times}_{eq}(x) = \Big\{ \left(d_i - l_i w_2^S\right)\ \left(d_i + l_i w_2^B\right) - \left(d_i + l_i w_2^S\right)\ \left(d_i - l_i w_2^B\right) \times e^{\dfrac{2x_B}{l_i}} + \left[\left(d_i + l_i w_2^B\right)\ l_i w_2^S - \left(d_i + l_i w_2^S\right)\ l_i w_2^B e^{\dfrac{x_B}{l_i}} \right] e^{\dfrac{x}{l_i}} + \left[\left(d_i - l_i w_2^B\right)\ l_i w_2^S\ e^{\dfrac{2x_B}{l_i}} - \left(d_i - l_i w_2^S\right)\ l_i w_2^B e^{\dfrac{x_B}{l_i}} \right] e^{-\dfrac{x}{l_i}} \Big\} \times \left[\left(d_i - l_i w_2^S\right)\ \left(d_i + l_i w_2^B\right) - \left(d_i + l_i w_2^S\right)\ \right]^{-1}, \tag{27}$$

and

$$\tilde{C}^{\times}_{R}(x) = \tilde{C}^{\times}_{R1}(x) + \tilde{C}^{\times}_{R2}(x), \tag{28}$$

where

$$\tilde{C}^{\times}_{R1}(x) = g_m \sqrt{\frac{\pi}{2}}\frac{\Delta R_{pd}}{2l_i}\ e^{\dfrac{\Delta R_{pd}^2 - 2l_i R_{pd} + 2l_i x_B}{2l_i^2}} \times \left[\left(d_i - l_i w_2^B\right)\ e^{\dfrac{x_B - x}{l_i}} + \left(d_i + l_i w_2^B\right)\ e^{-\dfrac{x_B - x}{l_i}} \right] \times \Bigg\{ \left(d_i + l_i w_2^S\right)\ e^{\dfrac{2R_{pd}}{l_i}} \times \left[\operatorname{erf}\left(\frac{\Delta R_{pd}^2 + l_i R_{pd} - l_i x}{\sqrt{2}\,\Delta R_{pd} l_i}\right) - \operatorname{erf}\left(\frac{\Delta R_{pd}^2 + l_i R_{pd}}{\sqrt{2}\,\Delta R_{pd} l_i}\right)\right] + \left(d_i - l_i w_2^S\right) \times \left[\operatorname{erf}\left(\frac{\Delta R_{pd}^2 - l_i R_{pd}}{\sqrt{2}\,\Delta R_{pd} l_i}\right) - \operatorname{erf}\left(\frac{\Delta R_{pd}^2 - l_i R_{pd} + l_i x}{\sqrt{2}\,\Delta R_{pd} l_i}\right)\right]\Bigg\} \times \left[\left(d_i - l_i w_2^S\right)\ \left(d_i + l_i w_2^B\right) - \left(d_i + l_i w_2^S\right)\ \left(d_i - l_i w_2^B\right)\ e^{\dfrac{2x_B}{l_i}} \right]^{-1}, \tag{29}$$

$$\tilde{C}^{\times}_{R2}(x) = g_m \sqrt{\frac{\pi}{2}} \frac{\Delta R_{pd}}{2l_i} e^{\dfrac{\Delta R_{pd}^2 - 2l_i R_{pd} - 2l_i x}{2l_i^2}} \left[d_i - l_i w_2^S + \left(d_i + l_i w_2^S\right) e^{\dfrac{2x}{l_i}} \right]$$

$$\times \left\{ \left(d_i + l_i w_2^B\right) e^{\dfrac{2R_{pd}}{l_i}} \times \left[\operatorname{erf}\left(\frac{\Delta R_{pd}^2 + l_i R_{pd} - l_i x_B}{\sqrt{2}\,\Delta R_{pd}\, l_i} \right) - \operatorname{erf}\left(\frac{\Delta R_{pd}^2 + l_i R_{pd} - l_i x}{\sqrt{2}\,\Delta R_{pd}\, l_i} \right) \right] \right.$$

$$\left. + \left(d_i - l_i w_2^B\right) e^{\dfrac{2x_B}{l_i}} \times \left[\operatorname{erf}\left(\frac{\Delta R_{pd}^2 - l_i R_{pd} + l_i x}{\sqrt{2}\,\Delta R_{pd}\, l_i} \right) - \operatorname{erf}\left(\frac{\Delta R_{pd}^2 - l_i R_{pd} + l_i x_B}{\sqrt{2}\,\Delta R_{pd}\, l_i} \right) \right] \right\}$$

$$\times \left[\left(d_i - l_i w_2^S\right) \left(d_i + l_i w_2^B\right) - \left(d_i + l_i w_2^S\right) \left(d_i - l_i w_2^B\right) e^{\dfrac{2x_B}{l_i}} \right]^{-1} . \tag{30}$$

It is interesting to note that for the 2D domain Eq. (16) represents the Helmholtz equation [8, 25]. One can obtain an analytical solution of this equation for the 2D case using the methods described in [8, 25]. However, this purpose is outside the scope of our investigation.

5 Analytical calculations

It was mentioned above that in the up-to-date electronics different layered structures such as $\mathrm{Ge_xSi_{1-x}}$/Si or silicon-on-insulator (SOI) are often used for decreasing the dimensions of a device and improving its performance. The derived analytical solution for a finite-length domain $[0, x_B]$ is convenient for modeling and investigating point defect diffusion in a separate layer of these structures. For example, in Fig. 1 the calculated distribution of point defects in a silicon layer of thickness 0.4 μm is presented. Primarily, the case of zero external radiation ($g_m = 0$) is considered for a better understanding of the influence of ion implantation.

It is evident that for zero fluxes of defects through the boundaries of the layer, the distribution of point defects is homogeneous and the value of normalized concentration of these defects is equal to 1 (dotted curve). Deviation from the uniform defect distribution occurs only if there are nonzero fluxes of defects through the boundaries or there is an absorption (generation) of point defects on the surface or at the interface. For example, the distribution of defects presented in Fig. 1 is calculated under the assumption that two fluxes of point defects through the left and right boundaries are directed along the x axis. For this purpose the coefficients w_2^S and w_2^B have been presented in the following form:

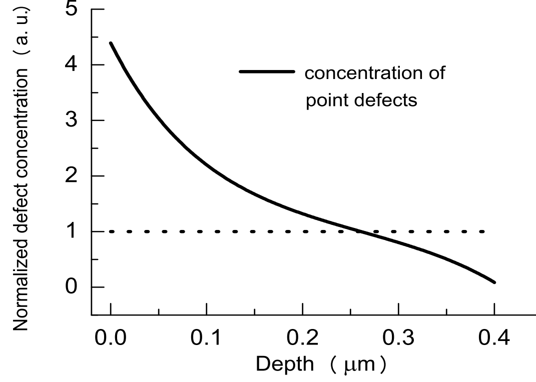

Figure 1: Calculated concentration distribution of the neutral point defects in a silicon layer of thickness 0.4 μm. The dotted curve represents the thermally equilibrium value of the normalized concentration of neutral point defects

$$w_2^S = \mathrm{v}_{eff}^S, \qquad w_2^B = -\mathrm{v}_{eff}^B, \tag{31}$$

where v_{eff}^S and v_{eff}^B are the effective rate of point defect removal outside the layer through the left and right boundaries, respectively. For the defect distribution presented in Fig. 1, the values v_{eff}^S =-0.0094 μm/s and v_{eff}^B = 4.0 μm/s were used. Also, the value of the average migration length of point defects $l_i = 0.1$ μm and the value of intrinsic diffusivity $d_i = 0.01$ μm^2/s were chosen. It can be seen from Fig. 1 that according to the boundary conditions (31) used for solving Eq. (16) the concentration of the point defects in the vicinity of the left boundary increases due to the supply of additional defects in the layer, whereas near the right boundary the concentration of intrinsic point defects decreases due to the removal of this species outside the layer. The analytical solution obtained describes the distribution of the concentration of point defects in the neutral charge state. The concentration of the charged defect species $C^r(x)$ can be calculated from the above-mentioned expressions $C^{Vr} = \tilde{C}^{V\times} C_{eq}^{V\times} h^{Vr} \chi^{-zz^{Vr}}$ and $C^{Iq} = \tilde{C}^{I\times} C_{eq}^{I\times} h^{Iq} \chi^{-zz^{Iq}}$ that follow from the mass action law.

It is worth noting that due to the quasi-stationarity of the diffusion equation for point defects, exactly the same solution takes place for the Dirichlet boundary conditions with $\tilde{C}^{\times}(0) = \tilde{C}_S^{\times} = 4.393$ a.u. and $\tilde{C}^{\times}(x_B) = \tilde{C}_B^{\times} = 0.08689$ a.u. Here $\tilde{C}_S^{\times}$ and $\tilde{C}_B^{\times}$ are the normalized concentrations of

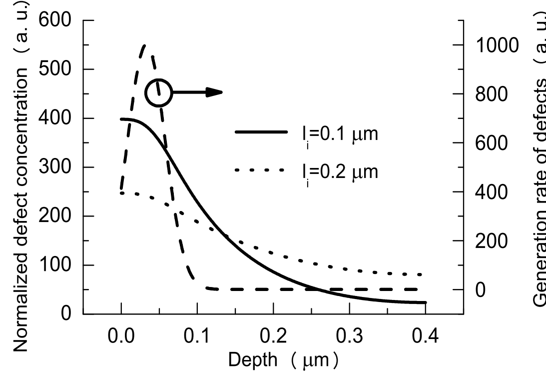

Figure 2: Concentration distribution of the neutral point defects normalized to the thermally equilibrium value of defect concentration in a silicon layer of thickness 0.4 μm for the case of hydrogen implantation with an energy of 2 keV. The dashed line represents the generation rate of point defects normalized to the equilibrium one

intrinsic point defects on the left (surface) and right boundaries of the layer.

Let us now consider the main features of the solutions of Eq. (16) in the case of intense generation of nonequilibrium point defects in the vicinity of the surface. Such generation can occur during low-energy implantation of hydrogen ions into the semiconductor substrate. For example, let us suppose that the energy of hydrogen implantation is 2 keV. Then, calculation performed by the code SRIM [34] gives the following values: $R_{pd} = 0.033$ μm, $\Delta R_{pd} = 0.0248$ μm, if one assumes that the distribution of generated defects is proportional to the distribution of implanted hydrogen ions.

In Fig. 2 the calculated concentration distribution of nonequilibrium point defects in a silicon layer of thickness 0.4 μm is presented. It was supposed that the maximal generation rate of point defects due to the ion implantation exceeds 1000 times the rate of thermal generation (g_m =1000), whereas the diffusion parameters are the same ($l_i = 0.1$ μm, $d_i =$ 0.01 μm^2/s). For comparison, the point defect distribution calculated for the value $l_i = 0.2$ μm is also presented. The case of zero fluxes through the left and right boundaries is investigated primarily. It follows from Fig. 2 that the point defect concentration decreases 1.6 times at the surface of a semiconductor if the average migration length increases 2 times. Simultaneously, the distribution of point defects becomes flatter. On the other hand, there is a significant increase in the point defect concentration, more

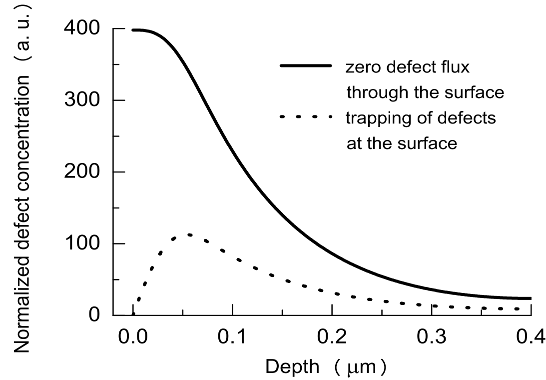

Figure 3: Concentration distribution of the neutral point defects normalized to the thermally equilibrium value of defect concentration in a silicon layer of thickness 0.4 μm for the case of hydrogen implantation with an energy of 2 keV. The solid line represents distribution of point defects calculated for the case of zero defect flux through the left boundary, whereas the dotted line describes diffusion of point defects under conditions of defect trapping on the surface

accurately by a factor of 3.4, on the right boundary of the layer.

Now, this paper investigates the main features of the solution obtained for the case of defect removal through the left boundary of the layer. It was mentioned above that this boundary condition is also similar to defect trapping on the surface of a semiconductor. For this purpose Fig. 3 presents two distributions of defects which were calculated for the case of zero defect flux through the left boundary and for the case of intensive trapping of defects by the surface, respectively. It is supposed that the average migration length of point defects is equal to 0.1 μ m. It can be seen from Fig. 3 that the trapping of point defects on the surface results in the change of the form of its concentration profile and in the significant decrease of defect concentration. For example, the maximal concentration of point defects decreases 3.5 times.

More serious influence of the surface on the distribution of point defects can be observed for small values of implantation energy. This is seen from Fig. 4, where a similar calculation for the energy of implantation of hydrogen ions equal to 500 eV is presented. For this value of hydrogen implantation energy the calculation of the parameters describing the distribution of implanted ions gives the following values: $R_{pd} = 0.0097$ μm,

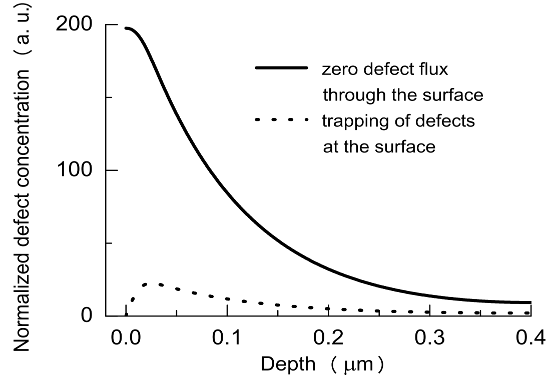

Figure 4: Concentration distribution of the neutral point defects normalized to the thermally equilibrium value of defect concentration in a silicon layer of thickness 0.4 μm for the case of hydrogen implantation with an energy of 500 eV. The solid line represents distribution of point defects calculated for the case of zero defect flux through the left boundary, whereas the dotted line describes diffusion of point defects under conditions of defect trapping on the surface

$\Delta R_{pd} = 0.011$ μm [34].

It can be seen from Fig. 4 that the maximal concentration of point defects decreases 8.8 times due to the trapping of point defects on the surface, which is in close vicinity (a few nanometers) to the region of intense generation of nonequilibrium point defects.

6 Numerical calculations

If the concentration of substitutionally dissolved impurity atoms is greater than n_i and intrinsic point defects can exist in different charge states, the coefficients in diffusion equations (9) and (10) represent the nonlinear functions of χ. In this case, Eqs. (9) and (10) can be solved only numerically. The finite-difference method [28] is used to find a numerical solution for Eqs. (9) and (10) in a one-dimensional (1D) domain $[0, x_B]$. Following Ref. [28], the first term on the left-hand side of these equations is approximated by a symmetric difference operator of second-order accuracy for the space variable x. To obtain the finite-difference operator, the integro-interpolation method was used. For this purpose, the uniform mesh with

the nodes $\{x_i\}$ $(i = 1, 2, \dots, k)$ is defined in the domain under consideration. The finite-difference operator was obtained by integrating the diffusion equation on the cells $\left[x_{i-\frac{1}{2}}, x_i, x_{i+\frac{1}{2}}\right]$ using the Newton-Cotes 3-Point Rule. This method allows one to obtain a convergent numerical solution. Finally, a set of the standard three-point equations has been obtained:

$$a_i^m \tilde{C}_{i-1}^{\times m} + b_i^m \tilde{C}_i^{\times m} + c_i^m \tilde{C}_{i+1}^{\times m} = f_i^m, \quad i = 2, 3, \dots, i_{k-1}, \tag{32}$$

where m is the iteration number.

To solve the set of the obtained nonlinear algebraic equations we use the simplest iterative technique, substituting the values of the neutral point defect concentration determined with the previous iteration into the coefficients of nonlinear algebraic equations (32). The same method was also used for boundary conditions. Because the built-in electric field does not influence diffusion of the neutral point defects directly, for the first iteration we used the uniform distribution of the neutral point defects $\tilde{C}_i^{\times 0} = 1$.

To approximate the boundary condition, the method of fiction domains is used [17]. For this purpose, we prolong a semiconductor and the solution domain beyond the left and right boundaries and introduce the fiction nodes x_0 and x_{k+1}. The symmetric difference operators for the left and right boundary conditions have been obtained by integrating these conditions on the cells $\left[x_{+\frac{1}{2}}, x_1, x_{1+\frac{1}{2}}\right]$ and $\left[x_{k-\frac{1}{2}}, x_k, x_{k+\frac{1}{2}}\right]$, respectively. The three-point equations for the boundary conditions have the form

$$a_1^m \tilde{C}_0^{\times m} + b_1^m \tilde{C}_1^{\times m} + c_1^m \tilde{C}_2^{\times m} = f_1^m, \tag{33}$$

$$a_k^m \tilde{C}_{k-1}^{\times m} + b_k^m \tilde{C}_k^{\times m} + c_k^m \tilde{C}_{k+1}^{\times m} = f_k^m. \tag{34}$$

In a similar way the three-point equations approximating the diffusion equation on the nodes $i = 0$, $i = 1$, $i = 2$ and $i = k - 1$, $i = k$, $i = k + 1$ have been obtained:

$$a_1^m \tilde{C}_0^{\times m} + b_1^m \tilde{C}_1^{\times m} + c_1^m \tilde{C}_2^{\times m} = f_1^m, \tag{35}$$

$$a_k^m \tilde{C}_{k-1}^{\times m} + b_k^m \tilde{C}_k^{\times m} + c_k^m \tilde{C}_{k+1}^{\times m} = f_k^m. \tag{36}$$

It is clear from the described method which introduces the fiction domains that the boundary conditions are approximated by a symmetric difference operator of second-order accuracy as the diffusion equation.

Combining equations (33) and (35) and also combining (34) and (36), one can exclude the concentrations of point defects in the fiction points x_0

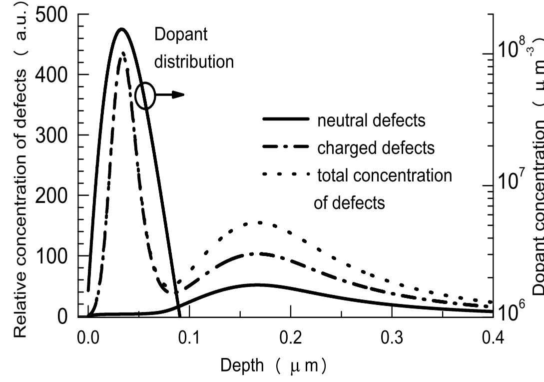

Figure 5: Concentration distribution of the neutral (solid curve) and singly charged (dot-dash curve) point defects normalized to the thermally equilibrium value of defect concentration for the case of hydrogen "hot" implantation with an energy of 10 keV. The temperature of substrate is equal to 800 °C

and x_{k+1}. Thus, the relationships between $\tilde{C}_1^{\times m}$ and $\tilde{C}_2^{\times m}$ and also between $\tilde{C}_{k-1}^{\times m}$ and $\tilde{C}_k^{\times m}$, required for the Gaussian elimination process [28], can be obtained.

To solve a set of the linearized three-point equations of the form of (32), the Gaussian elimination process for tridiagonal matrices was used, namely, the right elimination algorithm [28]. For each iteration, we control the stability of the elimination process. We also control the satisfaction of the point defect conservation law for the numerically generated solutions. Comparison for particular cases of the diffusion of point defects with the exact analytical solution obtained in this paper and calculations on meshes with different step sizes were carried out to verify the approximate numerical solution.

Figure 5 presents the results of numerical simulation of self-interstitial diffusion in a silicon layer doped by arsenic ion implantation with an energy of 10 keV. The Pearson distribution of type IV has been used to describe the arsenic concentration profile after implantation. The parameters of implantation taken from [5] are: $Q = 5{\times}10^{14}$ cm^{-2}; $R_p = 0.0363$ μm; $\Delta R_p = 0.014$ μm; $S_k = 0.6$. Here Q is the fluence of implanted ions, R_p and ΔR_p are the average projective range of implanted arsenic and straggling of the projective range, respectively, S_k is the skewness of impurity distribution after implantation. The calculated distribution of the dopant is presented

in Fig. 5 by a solid curve. It is supposed that generation of nonequilibrium point defects occurs due to the implantation of hydrogen ions with an energy of 10 keV. The following values of the parameters that describe hydrogen distribution after implantation have been used for modeling: $R_p = 0.1405$ μm; $\Delta R_p = 0.0503$ μm; S_k = -1.1; $R_m = 0.155$ μm. Here R_m is the position of the maximum of hydrogen distribution. It is supposed that the distribution of generated self-interstitials is proportional to the distribution of implanted hydrogen ions. The temperature of the semiconductor substrate is chosen to be 800 °C. This temperature is sufficient to provide the diffusion of defects to the surface and into the bulk of the silicon layer, but too low for arsenic redistribution. On the other hand, n_i is equal to 2.36×10^6 μm^{-3} for this temperature of "hot" hydrogen implantation and, therefore, χ reaches the maximal value 64.945 a.u. It results in a strong nonlinear dependence of the diffusivity of silicon self-interstitials. It is supposed that only neutral and singly negatively charged self-interstitials participate in diffusion. Therefore, to calculate the distribution of point defects, Eq. (10) is used with the concentration dependence of self-interstitial diffusivity:

$$d^I(\chi) = d_i^I d^I(\chi), \tag{37}$$

$$d_i^I = D_i^{I\times} + D_i^{I-} h_i^{I-}, \tag{38}$$

$$d^{IC}(\chi) = \frac{1 + \beta_1^I \chi}{1 + \beta_1^I}, \tag{39}$$

$$\beta_1^I = \frac{D_i^{I-} h_i^{I-}}{D_i^{I\times}}, \tag{40}$$

according to Ref. [31]. Here $D_i^{I\times}$ and D_i^{I-} are the diffusivities of neutral and singly negatively charged self-interstitials in undoped silicon, respectively; h_i^{I-} is a constant of local thermodynamic equilibrium for the reaction of transition of self-interstitials from the neutral charge state to the singly negatively charge state; β_1^I is the parameter describing a relative contribution of singly negatively charged self-interstitials to the defect diffusion in comparison with the neutral defects. It was supposed in the calculations presented that β_1^I is equal to 2 and the average migration length of silicon self-interstitials is chosen to be 0.1 μm.

It can be seen from Fig. 5 that the presence of nonuniform arsenic distribution significantly influences the diffusion of point defects. Indeed,

the concentration of charged silicon self-interstitials increases dramatically within the doped region and becomes approximately equal to the total defect concentration. This increase significantly enhances the diffusion flux of self-interstitials to the surface. As a result, a very low concentration of neutral point defects is observed in the implanted region. It is worth noting that for the undoped silicon layer the concentration of neutral point defects approaches zero only in the vicinity of the surface (see Fig. 4).

7 Conclusions

The analytical solution of the one-dimensional equation, which describes quasi-stationary diffusion of intrinsic point defects in semiconductor crystals, has been obtained for the case of the Robin boundary conditions on the left and right boundaries of the layer. It is supposed that the generation rate of nonequilibrium point defects is approximated by the Gaussian function. To derive an analytical solution of this boundary-value problem, the Green function approach has been used.

The solution obtained is focused on application in modeling technological processes used for fabrication of modern silicon integrated microcircuits and other semiconductor devices which have a layered structure. For example, it can be helpful for verification of the numerical solutions obtained and for investigation of the features of transport processes of vacancies and silicon self-interstitial atoms depending upon the implantation parameters and parameters of boundary conditions. It follows from a large uncertainty of the diffusivity and other transport properties of point defects known from the literature that the analytical solution obtained can successfully replace the numerical solution in modeling a number of technological processes used in the modern microelectronics.

To illustrate the usefulness of the solution obtained, the investigation of the changes in the form and concentration values of distribution of point defects has been carried out for different boundary conditions and two values of the average migration length of diffusing species. The cases of pure thermal generation of point defects within the limits of the layer and generation of nonequilibrium defects due to hydrogen ion implantation have been investigated. It has been shown that there is a strong influence of the surface on the concentration values and the form of distribution of nonequilibrium point defects when the implantation energy decreases.

The exact analytical solution obtained in this paper was used to verify the approximate numerical solution of diffusion equations for vacancies and self-interstitials. This numerical solution was applied to investigate the dif-

fusion of silicon self-interstitials in a highly doped surface region formed by ion implantation. It was shown that for such a structure a specific feature of the diffusion of nonequilibrium self-interstitials is the significant increase in the concentration of charged point defects in the highly doped region accompanied by the concentration of neutral point defects approaching zero.

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