DIFFERENT SHAPES OF IMPURITY CONCENTRATION PROFILES FORMED BY LONG-RANGE INTERSTITIAL MIGRATION

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Abstract. A model of interstitial impurity migration is proposed which explains the redistribution of ion-implanted boron in low-temperature annealing of nonamorphized silicon layers. It is supposed that nonequilibrium boron interstitials are generated either in the course of ion implantation or at the initial stage of thermal treatment and that they migrate inward and to the surface of a semiconductor in the basic stage of annealing. It is shown that the form of the “tail” in the boron profile with the logarithmic concentration axis changes from a straight line if the average lifetime of impurity interstitials is substantially shorter than the annealing duration to that bending upwards for increasing lifetime.

The calculated impurity concentration profiles are in excellent agreement with the experimental data describing the redistribution of implanted boron for low-temperature annealing at 750 Celsius degrees for 1 h and at 800 Celsius degrees for 35 min. Simultaneously, the experimental phenomenon of incomplete electrical activation of boron atoms in the “tail” region is naturally explained.

1 Introduction

The influence of the impurity diffusion mechanism on the form of dopant distribution after annealing of δ-doped layers has been investigated in [1, 2]. The authors obtained a one-dimensional analytical solution of the system of equations that includes the conservation law for the immobile component (substitutionally dissolved impurity atoms) and the diffusion equation for the mobile impurity component [1]. It was supposed that exchange of impurity atoms occurs between mobile and immobile species. It was also supposed that the initial impurity distribution is described by the δ-function and that the generation rate of mobile impurity interstitials is proportional to the concentration of substitutionally dissolved impurity atoms. It follows from the solution obtained that the extended “tail”, formed in the region of low impurity concentration of dopant profile after annealing, represents a straight line for the logarithmic concentration axis if the impurity atom migrates once. On the other hand, in the case of multiple events of migration of the interstitial impurity atom, the Gaussian distribution describes the shape of the impurity profile in the “tail” region.

As follows from the experimental data, after annealing the impurity concentration profiles can be similar to the Gaussian distribution. On the other hand, many of the measured impurity profiles, especially after low-temperature treatment, are characterized by an extended “tail” which looks like a straight line if the concentration axis is logarithmic (see, for example, the review of the experimental data in
Therefore, it was proposed in [1, 2] that the microscopic diffusion mechanism of impurity atoms be determined based on the form of the dopant distribution after annealing. It is worth noting that in [1, 2] continuous generation of mobile species in the region of high impurity concentration was supposed in the case where an impurity atom migrates once. In [4, 5] analytical solutions were obtained for the initial impurity distributions that, in contrast to [1, 2], represent a uniform doped layer or the Gaussian distribution. It was shown that the “tails” also represent a straight line just as for the initial distribution described by δ-function [1, 2].

At present, the method of ion implantation with low budget annealing such as, for example, high-temperature spice annealing or low-temperature long-term thermal treatment, is widely used for fabricating modern semiconductor devices and integrated microcircuits. During ion implantation, a fraction of the implanted ions can occupy an interstitial position and participate in the interstitial migration at subsequent annealing. It is expected that this phenomenon will be most pronounced for implantation of light ions, for example, boron ions, and also for implantation of the medium doses of heavier ions (∼10^{14} cm^{-2}) when the maximal concentration of impurity atoms is below the solubility limit but higher than the intrinsic carrier concentration at the annealing temperature [6]. Indeed, in these two cases one does not observe the amorphization of an implanted layer. As a result, annealing of defects generated by ion implantation occurs during the total thermal treatment, instead of the solid phase recrystallization of the created amorphous layer at the initial stage of the thermal processing. Indeed, it is well known that during solid phase epitaxial regrowth (SPER) there occurs annealing of the main part of defects created by ion implantation. In addition, almost all implanted impurity atoms go over into the substitutional position, even for the concentration above the solubility limit. It will be expected that in the absence of SPER the impurity atoms that remained in the interstitial position will migrate to a significant distance before they become substitutionally dissolved. It is worth noting that in the case of low-temperature treatment with duration of ten minutes and longer, a significant number of the impurity interstitials can also be generated at the initial stage of thermal processing due to annealing or rearrangement of different kind of defects incorporating impurity atoms.

Therefore, in contrast to the case of continuous generation of impurity interstitials during annealing described in [1, 2, 4, 5], the purpose of this work is to investigate the characteristic features of ion-implanted impurity redistribution that can appear due to diffusion of the previously formed interstitial impurity atoms.

2 The system of the equations describing interstitial diffusion

Let us assume that the substitutionally dissolved impurity atoms, as well as the impurity atoms incorporated into clusters, precipitates, and radiation defects are immobile and do not participate in diffusion due to the low annealing temperature. As the formation of extended “tails” due to the migration of impurity interstitials occurs in the region of low impurity concentration \( C \leq n_i \), we neglect the influence of the
built-in electric field on the diffusion process. Here $C$ is the concentration of substitutionally dissolved impurity atoms and $n_i$ is the intrinsic carrier concentration. Then, the system of equations that was proposed in [7, 8] and that describes migration of nonequilibrium impurity interstitial atoms and their subsequent transition to the substitutional position can be presented in the form given below.

1. The conservation law for substitutionally dissolved impurity atoms:

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

2. The equation of diffusion for nonequilibrium impurity interstitials:

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

where $C^{AI}$ is the concentration of nonequilibrium interstitial impurity atoms (IIA); $d^{AI}$ and $\tau^{AI}$ are the diffusivity and average lifetime of these impurity interstitials, respectively; $G^{AIR}$ is the generation rate of interstitial impurity atoms per unit volume due to the annealing of implantation defects and rearrangement of clusters (precipitates). It is worth noting that the total concentration of impurity atoms $C_T$ includes concentrations of the substitutionally dissolved impurity atoms, impurity atoms incorporated into clusters, precipitates, and radiation defects, as well as the concentration of impurity interstitial atoms $C^{AI}$.

It is well known that interstitial impurity atoms can become substitutionally dissolved due to the recombination with vacancies (the so-called the Frank-Turnbull diffusion mechanism [9]). In addition, a migrating interstitial impurity atom can kick-out the host atom and occupy a substitutional position (the reverse Watkins effect). Then, the average lifetime of IIA can be presented in the following form:

$$\frac{1}{\tau^{AI}} = k^{AV} C^V + k^{AI},$$  \hspace{1cm} (3)

where $k^{AV}$ is the effective coefficient of recombination of interstitial impurity atoms with vacancies; $C^V$ is the vacancy concentration; $k^{AI}$ is the coefficient describing transition of the interstitial impurity atom to the substitutional position due to the kick-out mechanism.

It is worth noting that this paper investigates an extreme case of the redistribution of implanted atoms occupying interstitial position immediately after implantation. Therefore, the generation term $G^{AIR} = 0$. Then, Eqs. (1) and (2) are independent if the vacancy distribution is uniform ($C^V(x, t) = \text{const}$). If $d^{AI}$ is also constant, one can obtain an analytical solution of Eq. (2).

3 Analytical solution of nonstationary diffusion equation for interstitial impurity atoms

An analytical solution of Eq. (2) can be obtained within the framework of the Green function approach [10, 11, 12]. For this purpose let us present Eq. (2) in the following form:
\[ \frac{\partial C^{AI}}{\partial \theta} = l_{AI}^2 \frac{\partial^2 C^{AI}}{\partial x^2} - C^{AI}, \]

where \( l_{AI} = \sqrt{d^{AI} \tau^{AI}} \) is the average migration length of impurity interstitials; \( \theta = t/\tau^{AI} \) is the relative time.

Let us also assume that the distribution of nonequilibrium impurity interstitials after implantation and after rapid annealing of implantation defects incorporating impurity atoms is proportional to the distribution of the implanted atoms which can be approximately described by the Gaussian distribution. Then, the initial condition for impurity interstitials can be presented in the following form:

\[ C^{AI}_m(x, 0) = C^{AI}_m \exp \left[ -\frac{(x - R_p)^2}{2\Delta R_p^2} \right], \]

where \( C^{AI}_m \) is the maximal concentration of interstitial impurity atoms after implantation or at the initial stage of annealing; \( R_p \) and \( \Delta R_p \) are the average projective range of implanted ions and the straggling of the projective range, respectively.

Let us obtain an analytical solution of the diffusion equation for nonequilibrium impurity interstitials \( \text{(4)} \) in one-dimensional (1D) semiinfinite domain \([0, +\infty]\). For the sake of simplicity, the Dirichlet boundary condition can be imposed on the surface and in the bulk of a semiconductor:

\[ C^{AI}(0, \theta) = C^{AI}_S, \quad C^{AI}(+\infty, \theta) = 0, \]

where \( C^{AI}_S \) is the concentration of interstitial impurity atoms on the surface of a semiconductor.

For this purpose, let us consider Eq. \( \text{(4)} \) in the infinite domain \([-\infty, +\infty]\) and use separation of variables [10, 13] assuming that the required solution is a product of two functions, one of which depends only on the relative time \( \theta \), whereas the other is the function of only the spatial coordinate \( x \), i.e., \( C^{AI}(x, \theta) = T(\theta)X(x) \). Then, \( C^{AI}_\theta = T'X, \quad C^{AI}_{xx} = TX'' \) and Eq. \( \text{(4)} \) transforms into the equation:

\[ T'X = l_{AI}^2 TX'' - TX. \]

Dividing the right- and left-hand sides of Eq. \( \text{(7)} \) by \( (l_{AI}^2 TX) \), we obtain the following equation:

\[ \frac{T'}{l_{AI}^2 T} = \frac{X''}{X} - \frac{1}{l_{AI}^2} = -\lambda^{*2}, \]

where \( \lambda^{*2} \) is the parameter of division that depends neither on \( x \), nor on \( \theta \), i.e., represents a certain constant. Using this property of \( \lambda^{*2} \), one can obtain the following system of independent equations:

\[ T'/T = -l_{AI}^2 \lambda^{*2}, \]

\[ X'' + \lambda^2 X = 0, \]

where \( \lambda^2 = \lambda^{*2} - 1/l_{AI}^2 \).
The solution of Eq. (9) has the following form:

\[ T(\theta) = T_0 \exp \left[ -l_{AI}^2 \lambda^2 \theta \right], \tag{11} \]

where \( T_0 \) is the value of the function \( T(\theta) \) for the initial moment of annealing.

The solution of homogeneous equation (10) can be obtained by employing the standard substitution \( X(x) = A_0 e^{\alpha x} \), where \( A_0 \) and \( \alpha \) are some constants. Based on the obtained solutions of Eqs. (9) and (10) and using the procedure described in [10], it is possible to find the solution of the boundary value problem (4), (5), and (6) for zero boundary condition on the surface of a semiconductor, \( C_S^{AI} = 0 \). This solution has the following form:

\[ C_{Z=S}^{AI}(x, \theta) = \int_0^\infty G(x, \xi, \theta) C_0^{AI}(\xi) d\xi, \tag{12} \]

where \( G(x, \xi, \theta) \) is the Green function

\[ G(x, \xi, \theta) = \frac{1}{2\sqrt{\pi l_{AI}^2 \theta}} \left\{ \exp \left[ -\frac{(x-\xi)^2}{4l_{AI}^2 \theta} \right] - \exp \left[ -\frac{(x+\xi)^2}{4l_{AI}^2 \theta} \right] \right\}. \tag{13} \]

To obtain the required distribution of the concentration of impurity interstitials for nonzero condition on the surface of a semiconductor, it is necessary to combine expression (12) with the well-known solution of the boundary value problem (4), (6) with zero initial condition (5):

\[ C^{AI}(x, \theta) = C_{Z=S}^{AI}(x, \theta) + C_S^{AI} \left[ 1 - \text{erf}(\frac{x}{2\sqrt{l_{AI}^2 \theta}}) \right]. \tag{14} \]

A similar procedure can be used to obtain a solution for the reflecting boundary condition on the surface and zero Dirichlet boundary condition in the bulk of a semiconductor:

\[ \frac{\partial C^{AI}}{\partial x} \bigg|_{x=0} = 0, \quad C^{AI}(+, \theta) = 0. \tag{15} \]

This solution has the following form:

\[ C^{AI}(x, \theta) = \int_0^\infty G(x, \xi, \theta) C_0^{AI}(\xi) d\xi, \tag{16} \]

where the Green function is

\[ G(x, \xi, \theta) = \frac{1}{2\sqrt{\pi l_{AI}^2 \theta}} \left\{ \exp \left[ -\frac{(x-\xi)^2}{4l_{AI}^2 \theta} \right] + \exp \left[ -\frac{(x+\xi)^2}{4l_{AI}^2 \theta} \right] \right\}. \tag{17} \]

The explicit expressions for the integrals in (12) and (15) can be obtained using the modern software allowing symbolic computation, such as “Mathematica” [14], “Mathcad” [15], and others. Unfortunately, the expressions obtained are too lengthy to be presented in this paper.

The total concentration of impurity atoms after annealing can be calculated by Eq. (1). Integrating this equation, we obtain
\[
C(x, t) = \frac{1}{\tau_{AI}} \int_0^t C_{AI}(x, t) \, dt + C_0(x),
\]

(18)

where \(C_0(x)\) is the initial distribution of substitutionally dissolved impurity atoms at the initial stage of annealing that can be approximated by the Gaussian distribution:

\[
C_0(x) = C_m \exp \left[ -\frac{(x - R_p)^2}{2\Delta R_p^2} \right].
\]

(19)

Here \(C_m\) is the maximal concentration of substitutionally dissolved impurity.

Unfortunately, within the framework of the software for the above-mentioned symbolic computation it is not possible to obtain an explicit expression for integral (18) with \(C_{AI}(x, t)\) described by expression (14) or (16). Therefore, the calculation of integral (18) was carried out by an approximate numerical method using the quadrature formula (Gauss 16-point formula) [16, 17].

4 Simulation of the interstitial redistribution of boron implanted into silicon during low-temperature thermal treatments

In Fig. 1 the calculated profiles of ion-implanted boron after low-temperature annealing are presented which show the change in the shape of the low concentration “tail” formed due to the interstitial diffusion for different ratios between the average lifetime \(\tau_{AI}\) and the duration of thermal treatment \(t_{ann}\). It is supposed that silicon is implanted with 1 keV boron ions to a dose of \(1.8 \times 10^{13}\) ion/cm\(^2\) \((R_p = 0.0056 \mu m; \Delta R_p = 0.0038 \mu m)\) and then subjected to annealing with duration of 10 min at a temperature of 750 °C. The average migration length of nonequilibrium boron interstitials has been chosen to be equal to 0.08 \(\mu m\). It is clearly seen from Fig. 1 that if the average lifetime of impurity interstitials \(\tau_{AI}\) is significantly shorter than the annealing duration \(t_{ann}\), the “tail” in the boron concentration profile represents a straight line in the case of the logarithmic axis of concentration. With increase in the average lifetime \(\tau_{AI}\), the shape of the “tail” becomes convex upwards, being characterized by an increasing slope angle in the bulk of a semiconductor similar to the Gaussian distribution. Thus, the calculations presented in Fig. 1 show clearly that for nonzero initial distribution of interstitial impurity atoms the “tail” in the low concentration region of impurity distribution has the form of the Gaussian distribution even for one event of impurity interstitial migration if \(\tau_{AI} \geq t_{ann}\), whereas in the case of continuous generation of impurity interstitials it occurs only in the case of numerous events of interstitial migration [1, 2].

It follows from the experimental data that the “tail” in the boron concentration profile after low-temperature treatment of ion-implanted layer can have a shape of a straight line [19, 20, 21] as well as a convex form characteristic for the Gaussian distribution [6, 23, 22, 25] if the concentration axis is logarithmic. For example, in Fig. 2 the boron concentration profile is presented which was measured in [6] by a method of the secondary ion mass spectroscopy (SIMS). Both the p-type and n-type Czochralski grown (CZ) commercial silicon wafers with conductivities of 4-6 Ωcm were used. Boron was implanted at
Figure 1: Calculated boron concentration profiles after low-temperature thermal treatment of implanted silicon substrate for different ratios between the average lifetime $\tau^{Al}$ and the duration of annealing $t_{ann}$.

room temperature with an energy of 40 keV to a dose $Q$ of $3 \times 10^{14}$ cm$^{-2}$. SIMS profile of the implanted boron after annealing at 750 °C with duration $t_{ann} = 1$ h is presented in Fig. 2 by filled circles. It can be seen from Fig. 2 that the maximal boron concentration after implantation $C_m = 3.04 \times 10^7$ µm$^{-3}$ is near the limit of boron solubility in silicon $C_{sol} = 2.33 \times 10^7$ µm$^{-3}$ for a temperature of 750 °C [26].

According to [27], the boron diffusivity of substitutionally dissolved atoms $D_i$ for this temperature is equal to $2.658 \times 10^{-10}$ µm$^2$/s. Then, for the thermal treatment for 1 h the characteristic diffusion length of impurity redistribution is $L_i = \sqrt{D_it_{ann}} = 9.78 \times 10^{-4}$ µm or it is approximately equal to 1 nm. On the other hand, it follows from Fig. 2 that the actual $L_i$ is approximately equal to 0.1 µm, i.e., 100 times longer. If we suppose that boron diffusion occurs due to the formation, migration, and dissociation of the “impurity atom – intrinsic point defect” pairs, it is necessary to accept that the average concentration of nonequilibrium point defects responsible for impurity diffusion is approximately $10^4$ times higher than the thermally equilibrium value. Not rejecting the possibility of such a strong radiation-enhanced diffusion, we shall carry out modeling of the redistribution of ion-implanted boron based on a more natural mechanism of migration of nonequilibrium impurity interstitials.

The following values of the model parameters were used to provide the best fit of the calculated boron concentration profile to the experimental one: The parameters prescribing the initial distribution of implanted boron: $Q = 3.2 \times 10^{14}$ cm$^{-2}$; $R_p = 0.145$ µm; $\Delta R_p = 0.042$ µm; the fraction of the
Figure 2: Calculated boron concentration profile (solid line) after thermal treatment of implanted silicon substrate at 750 °C for 60 min. Gaussian distribution (dotted line - total boron concentration and dashed line - concentration of interstitial boron atoms) was used to approximate the initial impurity profile. The dash-dotted curve represents interstitial boron after annealing. The experimental data (impurity distribution after annealing represented by filled circles) are taken from Ref. [6].

boron atoms in the interstitial position $p^{AI} = 34.2\%$. The parameters specifying the process of interstitial diffusion: the average migration length of boron interstitials $l_{AI} = 0.11 \mu m$. The reflecting boundary condition is imposed on the surface of a semiconductor when describing diffusion of boron interstitials. It is also supposed that the average lifetime of nonequilibrium impurity interstitials $\tau^{AI}$ is equal to the duration of annealing $t_{ann} = 1$ h. It is worth noting that the parameters prescribing the initial distribution of implanted boron is approximately equal to the values tabulated in [18]: $R_p = 0.131 \mu m; \Delta R_p = 0.0451 \mu m; S_k = -0.8 \mu m; R_m = 0.143 \mu m$, where $S_k$ and $R_m$ are respectively the skewness and the position of a maximum of impurity distribution as implanted which is described by the Pearson type IV distribution [18].

It can be seen from Fig. 2 that there is an excellent agreement between the calculated total boron concentration profile and boron profile measured by SIMS. A little difference in the near surface region follows from the assumption about the reflecting boundary for boron interstitials. In point of fact part of impurity interstitials cross over the surface of a semiconductor.

The modeling results of interstitial diffusion of ion-implanted boron during a low-temperature annealing at a temperature of 800 °C for 35 min are presented in Fig. 3. The experimental data of [23] were
used for comparison. In the Ref. [23] boron was implanted with an energy of 70 keV to a dose \( Q \) of \( 10^{15} \) cm\(^{-2}\). For the energy used in ion implantation, the parameters of the Pearson type IV distribution are: \( R_p = 0.219 \) µm; \( \Delta R_p = 0.0606 \) µm; \( S_k = -0.9 \) [18]. It is worth noting that for asymmetry \( S_k = -0.9 \) the position of a maximum of boron concentration \( R_m = 0.236 \) µm is close to the value \( R_p = 0.219 \) µm. It means that, just as in the previous case, one can neglect the asymmetry of impurity distribution and describe the boron profile after implantation, including the distribution of boron atoms in the interstitial position, by the symmetric Gaussian distribution [18–28].

The diffusivity of the substitutionally dissolved boron atoms \( D_i \) is equal to \( 1.928 \times 10^{-9} \) µm\(^2\)/s for a temperature of 800 °C [27]. Then, the characteristic diffusion length of impurity redistribution \( L_i = \sqrt{D_i t_{ann}} = 2.01 \times 10^{-3} \) µm or approximately 2 nm for thermal treatment during 35 min. On the other hand, it can be seen from Fig. 3 that the actual value of \( L_i \) is approximately 0.1 µm, i.e., 50 times longer. To provide this value of \( L_i \), the time-average concentration of the nonequilibrium point defects responsible for the impurity diffusion should be \( 2.5 \times 10^3 \) times higher than a thermally equilibrium value. It is necessary to note that in the case of radiation-enhanced diffusion of impurity atoms, due to the formation, migration, and dissociation of “impurity atom – intrinsic point defect” pairs, all impurity atoms in the “tail” region should be substitutionally dissolved, i.e., to be electrically active. However, the experimental data of [23] show that the significant fraction of boron atoms is electrically inactive in the “tail”. This phenomenon is easily explained within the framework of the interstitial diffusion mechanism described above if the lifetime of the interstitial boron atoms \( \tau^{AI} \) is near or longer the annealing duration \( t_{ann} \). Indeed, it follows from the later condition that a significant part of boron atoms are staying in the interstitial position, i.e. they are electrically neutral.

The following values of the model parameters were used to provide the best fit of the calculated boron concentration profile to the experimental one (see Fig. 3): **The parameters prescribing the initial distribution of implanted boron**: \( Q = 1.12 \times 10^{15} \) cm\(^{-2}\); \( R_p = 0.24 \) µm; \( \Delta R_p = 0.054 \) µm; the fraction of the boron atoms in the interstitial position \( p^{AI} = 26.5 \% \). It can be seen in Fig. 3 that the maximal boron concentration after implantation \( C_m = 8.3 \times 10^7 \) µm\(^{-3}\) is more than 2 times higher than the limit of boron solubility in silicon \( C_{sol} = 3.431 \times 10^7 \) µm\(^{-3}\) for a temperature of 800 °C [20].

**The parameters specifying the process of interstitial diffusion**: the average migration length of boron interstitials \( l_{AI} = 0.14 \) µm. As in the previous simulation, the reflecting boundary condition is imposed on the surface of a semiconductor when describing diffusion of boron interstitials. The average lifetime of nonequilibrium impurity interstitials \( \tau^{AI} = 48.3 \) min is chosen to be longer than the duration of annealing \( t_{ann} = 35 \) min. It is worth noting that the parameters prescribing the initial distribution of implanted boron is approximately equal to the values listed in the above-mentioned tables [18].

It can be seen from Fig. 3 that there is excellent agreement between the calculated total boron concentration profile and boron profile measured by SIMS. It is interesting to note that the concentration of interstitial boron atoms is approximately equal to the total boron concentration at the end of the “tail”. It means that this part of the “tail” is electrically inactive that is also consistent with the experimental
This paper considers the diffusion of boron interstitial atoms generated either during ion implantation or at the initial stage of annealing. In this meaning the case of interstitial diffusion under consideration is opposite to the investigations of [1, 2, 4, 5] where continuous generation of impurity interstitials is supposed. It follows from the simulation results obtained (see Figs. 2 and 3) that the model of diffusion of previously generated boron interstitials allows one to explain the formation of “tails” in nonamorphized silicon layers during low-temperature annealing with duration of 1 h or shorter. On the other hand, some increase in the boron concentration in the “tail” region occurs for annealing duration of 21 h at 800 °C [23] in comparison with the simulated boron profile for 1 h annealing presented in Fig. 3. We suppose that the additional generation of boron interstitials for such long-time treatments occurs due to the annealing or rearrangement of clusters or radiation defects.

Figure 3: Calculated boron concentration profile (solid line) after thermal treatment of implanted silicon substrate at 800 °C for 35 min. Gaussian distribution (dotted line - total boron concentration and dashed line - concentration of interstitial boron atoms) was used to approximate the initial impurity profile. The dash-dotted curve represents interstitial boron after annealing. The experimental data (impurity distribution after annealing represented by filled circles) are taken from Ref. [23].
5 Conclusions

To explain the redistribution of ion implanted boron during low-temperature annealing of nonamorphized silicon layers, a model of interstitial impurity migration is proposed. In contrast to other models of interstitial diffusion, it is supposed that nonequilibrium boron interstitials are generated either during ion implantation or at the initial stage of annealing and migration inward and to the surface of a semiconductor during the basic stage of annealing. It was shown that such kind of interstitial diffusion results in a “tail” in the boron concentration profile which has a form of a straight line for the logarithmic concentration axis if the average lifetime of impurity interstitials $\tau_{AI}$ is significantly shorter than annealing duration $t_{ann}$ and becomes convex upwards similar to the Gaussian distribution with increasing $\tau_{AI}$.

The calculated impurity concentration profiles are in excellent agreement with the experimental data that describe redistribution of implanted boron for low-temperature annealing at 750 °C for 1 h and at 800 °C for 35 min if $\tau_{AI}$ is equal to 1 h and to 48.3 min, respectively, i.e., the average lifetime of boron interstitials is equal or rather longer than the duration of annealing. The average migration length of impurity interstitial atoms is equal to 0.11 $\mu$m and to 0.14 $\mu$m for the annealing at temperatures 750 and 800 °C, respectively. The simulation results also show that 34.2 % and 26.5 % of the implanted boron atoms occupy interstitial position at the initial stage of annealing.

It is worth noting that the experimental phenomenon of incomplete electrical activation of boron atoms in the “tail” region is naturally explained within the framework of the model proposed. This fact and the excellent agreement with the measured boron profiles give evidence in favor of the model considering the formation of the main part of boron interstitials generated either during ion implantation or at the initial stage of annealing if we deal with low-temperature treatment of nonamorphized silicon layers.

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