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The reverse simulation models for target parameters

Yijun Zheng, Lin Pu, Yu Min and Juyan Xu

Abstract
Traditional forward simulation, such as SUPREM developed by Stanford University for implantation simulation is of low efficiency. Moreover, it is not able to quantitatively simulating some special distribution, such as the distribution of the maximum concentration gradient at the PN junction depth (X_J) or the quasi-rectangular distribution for material structure modifications. This paper proposes a reverse simulation model for target parameters, which use reverse deduction from expected values and the mathematic method of solving the conditional extremum of multivariable functions. The Implantation Parameters Quantitative and One-shot reverse simulating (IPQORS) the special distribution have been studied in this article. Research results indicate that IPQORS is feasible.

Keywords: Forward simulation; SUPREM; Reverse simulation.

1. Introduction
The LSS theory (Lindhand, Schanff and Scliatt) laid a sound foundation for the implantation forward simulation such as SUPREM [1] by Stanford University. SUPREM has been optimized and upgraded in many versions, e.g. SUPREM-Ⅱ [2], SUPREM-Ⅲand Suprem-Ⅳ [3]. In nearly half a century, Ion implantation doping and its distribution have been the research foundation of semiconductor devices, integrated circuit (IC) [4-6] and material structure modification. Today, Ion implantation has become one of the most important technologies of IC industry. Moreover, implantation has significant applications in material modification such as multi-energy dose implanting of O^+、Ge^+ and C^+ into a Si substrate with a quasi-rectangular distribution, which can form the SIMOX SOI, the $Si_{1-x}Ge_x$ and the $Si_{1-y}C_y$, respectively.
A forward simulation is started by empirically choosing a set of energy/dose data based on the parameters of aided process such as the mat oxide (SiO_2) thickness (T_{OX}), substrate concentration (C_{SUB}) and high temperature (D) duration T (DT or Dt). If simulation results do not match the expected values, the input data are adjusted and the simulation is repeated until satisfactory results are obtained. The process of determining the energy/dose for a single implantation is time-consuming. It becomes worse for a multi-energy dose implantation for special distributions such as the distribution of the maximum concentration gradient at the PN junction depth (X_J) and the quasi-rectangular distribution for material modifications. Even if a large amount of work is spent on the forward simulation. It is difficult to determine whether the concentration gradient distribution at X_J is the maximum, this is an inherent weakness of traditional forward simulation. This paper introduces a reverse simulation method, called IPQORS. It is based on C_{SUB}, X_J', $R_{\square}$, T_{OX}, and DT, first finds a feature point that represents the DT's distribution parameters, then deduces the mathematical expression. Finally, a single implantation target parameter can be obtained and is also based on C_{SUB}, X_J', $R_{\square}$, T_{OX}, DT, and the requirement of the maximum concentration gradient at X_J and quasi-rectanglized, by solving the mathematical equation built from the DT's distribution parameters. In this way, a multi-energy/dose implantation target parameter can be obtained with Quantitative and One-shot.

2. Modules and mode
2.1 Modules
In Table 1, there are different types of choices including the energy category, the number of implantations and the mode of implantation.

The four basic modules are marked by √ and √, and the others are marked by ←and '←. The relationship between the energy within 20 keV ~ 200 Kev and the mean projection range (R_P) with standard deviation (σ_p) follows LSS theory, while the energy below 20 keV [7] follows Molecular Dynamics (MD). Although two models are based upon here, both their implantation distributions are quasi-normal.

2.2 Models

The following four basic models cover the twelve modules in Table 1.

Model. 1: Single energy/dose is implanted in Si through SiO_2 (Poly-Si) and followed by annealing and a post-high temperature (MHE S E/D I SiO_2/Si HT).

Model. 2: Double (Multiple) energy/dose are implanted in Si through SiO_2 (Poly-Si) and followed by annealing and a post-high temperature (MHE T E/D I SiO_2/Si HT).

Model. 3: Single energy/dose is implanted in Si through SiO_2 (Poly-Si) and followed by shucking off SiO_2, re-oxidation and a post-high temperature (MHE S E/D S O SiO_2 R O HT).

Model. 4: Double (Multiple) energy/dose are implanted in Si through SiO_2 (Poly-Si) and followed by shucking off SiO_2, re-oxidation and a post-high temperature (MHE T E/D S O SiO_2 R O HT).

2.2.1 Model. 1: MHE S E/D I SiO2/Si HT

As shown in Figure 1, the implantation quasi-normal distribution which has a peak R (R_P) and standard deviations σ_{P1} and σ_{P2}. It changes to the DT's quasi-normal distribution, which has the parameters R', σ_1' and σ_2' (Note that IPQORS does not consider the skewness (S) and kurtosis (K) of the meticulous parameter in four moments of Pearson-IV model. It focuses on adjusting the distribution parameters, D_β and σ_t *et al.* to achieve the precision of the SUPREM modeled by Pearson-IV). The final distribution of the implanted B in Si and SiO_2 at the Si/SiO_2 interface after high temperature is discontinuous. X_J' and $R_\square$, which is enclosed by the distribution points Q_1', P_t, Q_2' and X_J', are formed. TC is the decreased thickness when SiO_2 transforms into Si. SiO_2 ranges from 0x to 0 and Si ranges from 0 to ∞. The implantation distribution and the distribution after Dt can be represented by symmetric Gaussian distribution given in equations 1 and 2, respectively:

$$C(x, 0)=DS_{Si}/\sigma_P(2\pi)^{1/2}\exp[-(x-R_P)^2/2\sigma_P^2] \quad (1)$$

$$C'(x,t)=DS'_{Si}/\sigma_t(2\pi)^{1/2}\exp[-(x-r_t)^2/2\sigma_t^2] \quad (2)$$

Where DS_{Si}, DS'_{Si}, σ_t and r_t are the implantation dose in Si, the D_t's re-distribution dose in the Si, the D_t's standard deviation and the peak location, respectively. The σ_P and σ_t can be substituted by the quasi-normal distribution parameters σ_{P1}, σ_{P2}, and σ_{t1}, σ_{t2}, respectively.

Lemma 1: Similar to a normal distribution function, finding the partial derivatives of the quasi-normal distribution function with respect to x, DS'_{Si} and r_t, is not influenced. This is because σ_P, σ', and σ_t are parameters rather than independent variables like x, DS'_{Si} and r_t. The σ_{P1}, σ_{P2}, σ_{t1}, σ_{t2}, and σ_1' σ_2' are discussed in details below.

Lemma 2: DT can be expressed by the diffusion coefficients D_1 and D_2 at the spots Q_1 and Q_2 respectively. Such as σ_{p1} σ_{p2}, σ_{t1} σ_{t2}, $\sigma_1'^2$ $\sigma_2'^2$, D_{eff} and D_{Si} can be expressed as the following:

$$\sigma_p= \gamma\sigma_{p1}+\omega\sigma_{p2}$$
$$\sigma_1'^2=\sigma_{p1}^2+D_1T$$
$$\sigma_2'^2=\sigma_{p2}^2+D_2T$$
$$\sigma_{t1}^2=\sigma_{p1}^2+D_1t$$
$$\sigma_{t2}^2=\sigma_{p2}^2+D_2t$$

Table 1: The Modules and the Classification

Module / Type / Mode	Mid-high Energy Single	Mid-high Energy Twice	Low Energy Single	Low Energy Twice
Implant in Si Through SiO_2, Followed by Anneal	√ MHE S E/D I SiO2/Si HT	√ MHE T E/D I SiO2/Si HT	← LE S E/D I SiO2/Si HT	← LE T E/D I SiO2/Si HT
Implant in Si Through SiO_2, Suck off SiO_2, re-Oxide, Post-High temperature	√ MHE S E/D S O SiO2 R O HT	√ MHE T E/D S O SiO2 R O HT	← LE S E/D S O SiO2 R O HT	← LE T E/D S O SiO2 R O HT
Implanting in Si Oxidation, Post-High Temperature	↑ MHE S E/D ID SiO2 HT	↑ MHE T E/D ID SiO2 HT	↖ LE S E/D ID SiO2 HT	↖ LE T E/D ID SiO2 HT

$$\sigma_t = (\gamma\sigma_{t1}+\omega\sigma_{t2})$$
$$D_1=\alpha D_{eff}+\beta D_{si}$$
$$D_2=\alpha D_{si}+\beta D_{eff},$$

where σ_{p1} and σ_{p2} are the standard deviations of the quasi-symmetry distribution implantation; D_{eff} and D_{Si} are the impurity diffusion coefficients of the diffusion into SiO_2 and Si, respectively.

The α and β are discussed below.

Proof: If α =1 and β= 0, then $\sigma_1'=(\sigma_{p1}^2+D_{eff}\ T)^{1/2}$ and $\sigma_2'=(\sigma_{p2}^2+D_{Si}T)^{1/2}$, which means that both D_{eff} and D_{si} are contributed to the standard deviations σ_1' and σ_2' but the peak value position does not move. This is not possible. Thus, α=1 and β= 0 cannot be true. Similarly, α=0 and β= 1 cannot be true neither. Thus, α has to decrease gradually from '1' and β increase gradually from '0'. In this way, the contributions of D_{eff} and Dsi to moving the peak value position are increased and they are dominant until α< 0.5 and β > 0.5. On the contrary, when α > 0.5 and β< 0.5, the contributions of D_{eff}

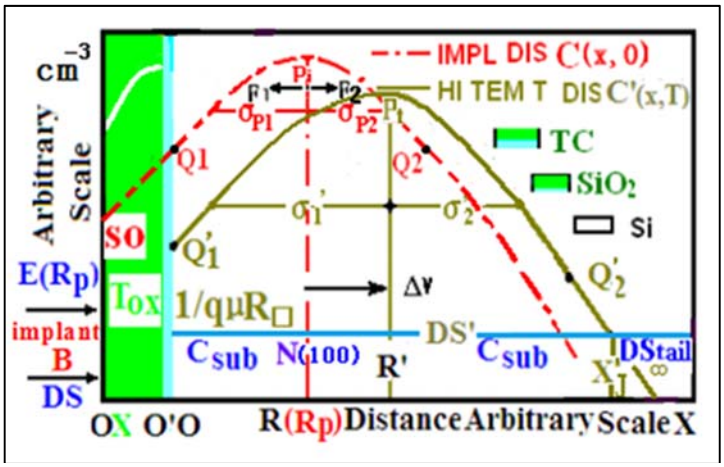

Fig 1: The quasi-normal distribution of Boron ions implanted by single Energy/Dose (R_p/DS) in Si through SiO_2 of thickness Tox and after high temperature DT.

and D_{Si} to the standard deviations σ_1' and σ_2' are dominant. The conclusion is that high temperatures not only drive the position of the peak value but also change σ_1' and σ_2' according to $\sigma_1' = (\sigma_{p1}^2 + D_1T)^{1/2}$ and $\sigma_2' = (\sigma_{p2}^2 + D_2T)^{1/2}$. The α and β are determined during verification, depending on different impurities, the high temperature atmosphere and an implantation pattern. A modulation starts from α=0. 5 and β=0. 5. The γ and ω are similar to α and β.

2.2.1.1 Reverse Simulation of the R_P (corresponding to E)

The distribution of implanted dopants after a high temperature processing should be continuous and derivable at every distribution point. Q_1 and Q_2 are chosen as the feature points. It is assumed that the dopants will neither increase nor disappear. Under a high temperature Dt_j, dopant concentration of the peak value is between Q_1 and Q_2. The dopants diffused into SiO_2 and Si with the flux densities of F_{j1} and F_{j2} and the flux density rates of V_{j1} and V_{j2}. The flux density rate difference, i.e. $\delta v = V_{j1} - V_{j2}$, is determined by the effective diffusion coefficient in the respective direction at the spots Q_1 and Q_2, i.e. $\omega(1/m)D_{Si}$ and D_{Si}. Note that D_{Si} and ω are the Si effective diffusion coefficient and the effective coefficient of 1/m, respectively. Here $\omega(1/m)\ D_{Si}$ boosts the dopants diffusion into SiO_2 due to the segregation coefficient 'm' at the interface SiO_2/Si and thus $D_{eff} = \omega(1/m)D_{Si}$. The feature point Q_1 is always at the interface of SiO_2/Si. The location of Q_2 however varies. It cannot be determined by using the method as obtaining Q_1 from the equal distance of the symmetric line in the Gaussian distribution. Instead, it should be determined by the equivalent principle of the two sides quasi-flux density rate (quasi-rate), i.e.$\delta v' = 0$. The quasi-rate value multiplied by the diffusion coefficient is the flux density rate in the theory of traditional heat conduction and solid diffusion. Equation 4 below can be derived from equation 3 by deleting D_{eff} and D_{Si}. By solving it, the locations of feature points are obtained.

$$\delta v = -D_{eff}\,[\delta C'(x,t)/\delta x]/C'(x,t)_{x=q1j} - D_{Si}[\delta C'(x,t)/\delta x]/C'(x,t)_{x=q2j} \quad (3)$$

$$\delta v' = -[\delta C'(x,t)/\delta x]/C'(x,t)_{x=q1j} - [\delta C'(x,t)/\delta x]/C'(x,t)_{x=q2j} \quad (4)$$

Because $\delta v' = 0$, equation 5 is derived as the following:

$$-[\delta C'(x,t)/\delta x]/C'(x,t)_{x=q1j} = [\delta C'(x,t)/\delta x]/C'(x,t)_{x=q2j} \quad (5)$$

And equation 6 can be derived as the following:

$$q_{2j} = r_j\,(\sigma_{j1}^2 + \sigma_{j2}^2)\ /\ \sigma_{j1}^2 \quad (6)$$

In this way, the dopant flux densities, the flux density rates and the flux density rate difference at q_{1j} and q_{2j} can be represented as the following:

$$F_{2j} = D_{Si}\delta C'(x,t)/\delta x_{x=q2j} \quad (7)$$

$$F_{1j} = -D_{eff}\delta C'(x,t)/\delta x_{x=q1j} \quad (8)$$

$$V_{2j} = F_{2j}/C'(x_{q2}, t_j) = D_{si}\,(r_j - x_{q2j})\ /\sigma_{j2}^2 = D_{si}\,(r_j - q_{2j})/\ \sigma_{j2}^2 = D_{Si}\,[r_j - r_j\,(\sigma_{j1}^2 + \sigma_{j2}^2)\ /\sigma_{j1}^2]\ /\ \sigma_{j2}^2 \quad (9)$$

The subscript 2 in σ_{j2}^2 denotes the inner direction of the Si and the subscript 1 in σ_{j1}^2 denotes the direction of the SiO_2.

$$V_{1j} = -\,F_{1j}\ /C'(x_{q1}, t_j) = -\,D_{eff}\,(r_j - x_{q1j})/\ \sigma_{j1}^2 = -D_{eff}\,(r_j - q_{1j})\ /\sigma_{j1}^2 \quad (10)$$

$$\delta v = V_{1j} - V_{2j} = -F_{1j}\ /C'(X_{q1}, t_j) - F_{2j}\ /\ C'(x_{q2}, t_j) = -D_{eff}\,(r_j - q_{1j})/\ \sigma_{j1}^2 - D_{Si}\,(r_j - q_{2j})\ /\sigma_{j2}^2 = r_j\ (D_{Si} - D_{eff})\ /\sigma_{j1}^2 \quad (11)$$

In equation 11, r_j is the peak location of the quasi-normal distribution at the high temperature Dt_j, which transforms equation 11 into equation 12,

$$r_j = \delta v\sigma_{j1}^2\ /\ (D_{Si} - D_{eff}) \quad (12)$$

At the DT, r_T and δvcan be substituted by R' and Δv, respectively. According to the normal distribution, R' can be written as the following:

$$R' = X_J' - \sigma'[2\ln DS_{Si}'/\sigma'(2\pi)^{1/2}\ C_{SUB}]^{1/2} \quad (13)$$

As shown in Figure 1, the implanting dose DS' is bound by Q_1, P_j, Q_2 and X_J'. It can be expressed as the following:

$$DS' = 1/q\mu R_{\square} + X_J'C_{SUB} \quad (14)$$

where $1/q\mu R_{\square}$ is the dose in the inversion layer of the corresponding $R_{\square}$ and $X_J'C_{SUB}$ is the dose compensating the substrate. DS_{Si}' is solved below.

Lemma 1: Quasi-normal distribution in Figure 1. In addition to $\sigma_1 \neq \sigma_2$, the coordinates need to adjust the coordinates to make correspondence between 0 to ∞, the integral above and below the boundary, and to pay attention only to the implantation impurity distribution in the Si. Forcing (x-R') /σ'=δx on σ', the unit normalization generates a new standard deviation. In this way, the question turns the following:

$$DS_{si}' = \int_0^{(X_J-R')/\sigma'} C'(x, T)\,dx + \int_{(XJ-R')/\sigma'}^{\infty} C'(x, T)\,dx = DS' + \int_{(XJ-R')/\sigma'}^{\infty} C'(x, T)\,dx = DS' + DS_{tail} \quad (15)$$

Le Lemma 2: $\sigma_1' \neq \sigma_2'$ becomes unimportant due to integral. Let $\sigma_1' = \sigma_2' = \sigma'$, then DS_{Si}' can be expressed theoretically by equation 15. Table 2 is a quasi-normal distribution value table. It is transformed from the Standard Normal Distribution Value Table that is remodeled by the physical parameters of the ion implantation. The θ_δ is the ratio of DS_{si}'/DS.

Lemma 3: DT's reverse simulation starts from R' with a fixed step of 0.1 minutes. The n_{th} reverse iterative simulation can be expressed as

$$r_{(T-n\times 0.1)} = \delta v_{T-(n-1)\times 0.1}\ \sigma^2_{t1(T-n\times 0.1)} / [D_{si\ (T-n\times 0.1)} - D_{eff\ (T-n\times 0.1)}] = r_{T-(n-1)\times 0.1}(D_{si\ T-(n-1)\times 0.1} - D_{eff\ T-(n-1)\times 0.1}) / \sigma^2_{tj1\ T-(n-1)\times 0.1} \times \sigma^2_{t1\ (T-n\times 0.1)} / [D_{si\ (T-n\times 0.1)} - D_{eff\ (T-n\times 0.1)}] \quad (16)$$

Iterations are performed until achieving R in Si. The mat SiO_2 thickness before implantation is converted to the Si thickness according to the blocking ability of the implanting ions (in fact, according to the material density). Then, the required implanted energy can be obtained according to the expression below:

$$R_p = R + T_{OX}k \quad (17)$$

where T_{OX} is the thickness of mat SiO_2 before implantation; k is the density ratio of SiO_2 to Si.

2.2.1.2. Reverse Simulation of the DS (implantation dose)
The distribution of implanted dopants in Si after DT is:

$$C'(x,T) = [DS_{Si}'/(2\pi)^{1/2}\sigma']\exp[-(x-R')^2/2\sigma'^2] \quad (18)$$

where DS_{Si}' is the total dose in Si at the final DT. As discussed above, DS_{Si}', which is called as conditional dose, is determined by DS'. According to equation 2, DS_{Si}' at the high temperature Dt can also be called as the course dose. The corresponding peak concentration, C_{PT}, is expressed as $C_{PT} = DS_{si}'/(2\pi)^{1/2}\sigma'$ and can be changed to the following:

$$DS_{Si}' = C_{PT}(2\pi)^{1/2}\sigma' \quad (19)$$

Starting from DS' by using a fixed step of 0.1 minutes, the n_{th} reverse iterative simulation can be expressed as

$$DS_{si\ (T-n\times 0.1)}' = C_{PT\ T-(n-1)\times 0.1}(2\pi)_{1/2}\sigma'_{(T-n\times 0.1)}$$

Table 2: The Table of quasi-normal distribution value

δ x	θδ	DS_{Si}' (DS/θδ)	δ x	θδ	DS_{Si}' (DS/θδ)	δ x	θδ	DS_{Si}' (DS/θδ)	δ x	θδ	DS_{Si}' (DS/θδ)
0.0	0.5	2.0	0.8	0.788	1.26904	1.9	0.971	1.02987	2.7	0.996	1.00402
0.1	0.54	1.85	0.9	0.816	1.22549	2.0	0.977	1.02354	2.8	0.997	1.00301
0.2	0.579	1.72712	1.0	0.841	1.18906	2.1	0.982	1.01833	2.9	0.998	1.002
0.3	0.618	1.61812	1.1	0.864	1.15741	2.2	0.986	1.0142	3.0	0.9987	1.00135
0.4	0.655	1.52672	1.2	0.885	1.12994	2.3	0.989	1.01112	3.2	0.9993	1.00069
0.5	0.692	1.44509	1.3	0.903	1.10742	2.4	0.992	1.00806	3.4	0.9997	1.00034
0.6	0.726	1.37741	1.4	0.919	1.08814	2.5	0.994	1.00604	3.6	0.9998	1.00016
0.7	0.758	1.31926	1.5	0.933	1.07181	2.6	0.995	1.00503	3.8	0.9999	1.00002

$$= [DS_{si\ T-(n-1)\times 0.1}'/(2\pi)^{1/2}\sigma'_{T-(n-1)\times 0.1}](2\pi)^{1/2}\sigma'_{(T-n\times 0.1)} = [DS_{si\ T-(n-1)\times 0.1}'/\sigma_{T-(n-1)\times 0.1}]\sigma'_{(T-n\times 0.1} \quad (20)$$

Equation 20 is performed until the total dose DS_{Si}' in Si is reached. Then the thickness of mat SiO_2 is transformed into thickness of the Si. Finally, according to the Table 2 to calculate the total dose implantation DS. In this way, model 1 is formed. The target parameter of a single implantation (R_P/DS) can be simulated reversely.

2.2.2 Model. 2: MHE T E/D I SiO2/Si HT
C'(x, T) is marked by the solid line in Figure 2. It is the distribution piled by two implantation distributions, $C_1'(x, T)$ and $C_2'(x, T)$ after the DT. Twice implantation should meet not only the requirement of C_{SUB}, Tox, DT, X_J' and $R_{\square}$, but also the distribution requirement of having the maximum concentration gradient at X_J' and being in a quasi-rectangular form. Corresponding to this physical picture, it is a problem of finding a conditional extremum of multivariable functions. Thus, we come up with the following mathematical expressions.
Suppose

$$U(DS'_{1Si}, DS'_{2Si}, R'_1, R'_2) \text{ and } DS'_{1Si} = DS'_{Si} - DS'_{2Si}$$

Then,

$$U\ (DS'_{2Si}, R'_1, R'_2) = \delta C'(x,t)/\delta x = \delta[C_1'(x,t) + C_2'(x,t)]/\delta x \quad (21)$$

$$V = [C_1'(x_j,t) + C_2'(x_j,t)] - C_{SUB} \quad (22)$$

$$F(U, V) = U + \lambda V \quad (23)$$

Equation 21 is an objective function and equation 22 is a conditional function. Equation 23 is the mathematical expression of new conditional variable functions. DS'_{Si} is the total dose piled by twice implantation in Si, which can be obtained from the DS'. It meets the requirement of C_{SUB}, Tox, DT, X_J' and $R_{\square}$ and satisfies the condition of the maximum concentration gradient at the X_J'(or interface of materials modification)

$$\delta F(x,t) / \delta DS_{2si} = 0 \quad (24)$$
$$\delta F(x,t) / \delta_{R'1} = 0 \quad (25)$$
$$\delta F(x,t) / \delta_{R'2} = 0 \quad (26)$$
$$\delta F(x,t) / \delta\lambda = 0 \quad (27)$$

Next, partial differential equations is solved by first obtaining the general solutions of DS'_{2Si}, R'_1, R'_2 and λ and then the specific solution of the physical picture of this model. After solving for R'_1, DS'_{1Si}, R'_2 and DS'_{2Si}, linear superposition and separation are used. Their implantation energy (R_1 and R_2) and dose (DS_{1Si} and DS_{2Si}) can be simulated as in model 1. Because the distribution of a finite implantation is not even, it is necessary to add a series of energy and dose to ensure the quasi-rectangular distribution. A subprogram needs to be introduced here for estimating the smoothness. If the standard deviation that comes from the previous computation does not match the predetermined standard deviation, additional implantations are needed until the requirement is met.

2.2.3 Model. 3: MHE S E/D S O SiO2 R O HT

This model can also be called as re-oxidation model. In

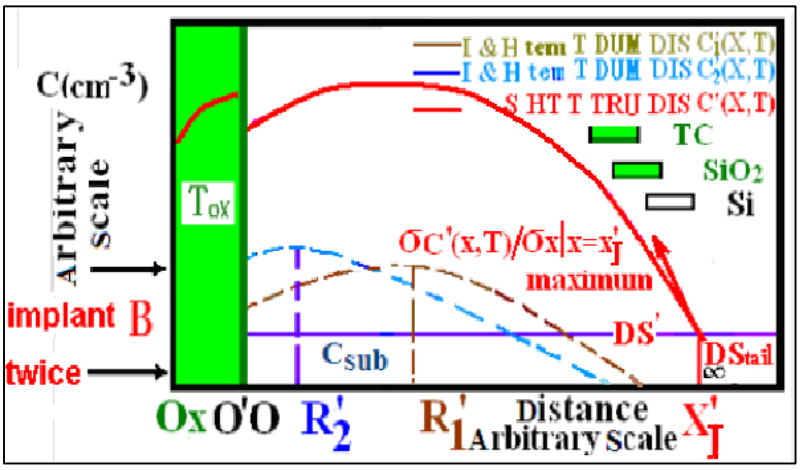

Fig 2: The distribution C'(x, T) of the boron ions when performing implantation twice in Si through SiO_2 with a thickness of Tox.

Figure 3, the vertical axis is concentration. The horizontal axis "X" corresponds to Si and the horizontal axis "Y" corresponds to SiO_2. The surface of the initial Si, the interface of SiO_2/Si at thermal oxidation t_1 and the interface of SiO_2/Si at the final thermal oxidation are denoted by a dash-dot line, a dotted line and a solid line in Figure 3, respectively. The distribution of dopants in Si after the thermal oxidation t_1 is denoted by C_1"(x, t_1). The distribution of dopants in Si and SiO_2 at the final thermal oxidation (T_1) are denoted by C_1"(x, T_1) and C_2"(y, T_1), respectively. The peak value location is denoted by R". The escaped dopants from the surface of Si during oxidation at time t_1 can be expressed as $D_2\delta C'(x,t_1)/\delta x$ x=0. After re-oxidation and high temperature processing, the escaped dopants in SiO_2 can be represented by D_1 δC"(y, t) / δx. Its solution is described in the next paragraph. Model 3 includes three parts: a) implantation in Si through SiO2; b) annealing, remove SiO2; c) re-oxidation followed by high temperature processing. The three parts are marked ''', '' and ', respectively. The third levelC_1'''(x, T_2) and C2'''(y, T_2) can be simulated as in model 1; The second level C_1"(x, T_1) and C_2"(y, T_1) are shown in Fig3. The first level C'(x, T) is shown in Fig.1. The following paragraph mainly discusses the second level C1"(x, T_1) and C2"(y, T_1).

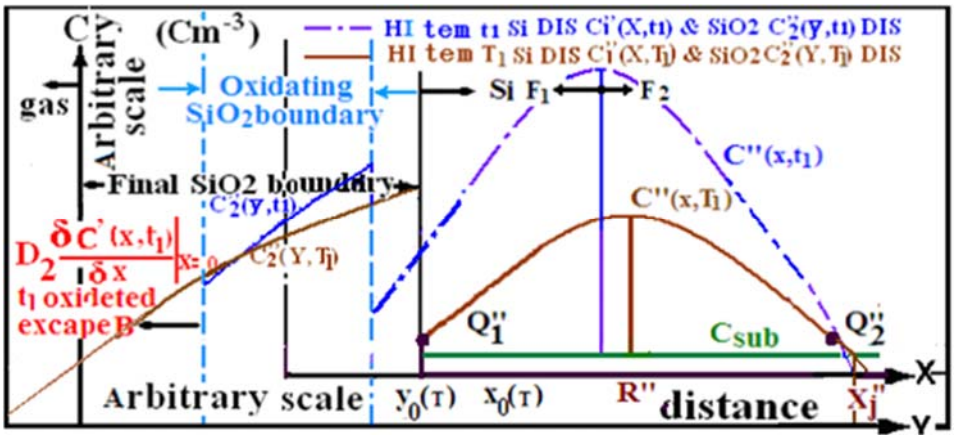

Fig 3: Quasi-normal distribution for after the re-oxidation

2.2.3.1 The Expression of the R'' in the Reoxidation Model

The re-oxidation model, which is based on model 1, needs to take into account the impacts of thermal oxidation on the shift of the peak location.

Remark 1: The oxidated SiO_2 is approximately 2.27 times as thick as the consumed Si. In other words, the capacity of the dopants of SiO_2 is approximately 2.27 times of that of Si. It can be deduced that the effective diffusion coefficient of Si that was intended to be oxidated into SiO_2 increases 2.27ω times, comparing to the original Si (where is the effective coefficient). The extra diffusion coefficient of the oxidated Si is 1/β, where 1/β=2.27ω. The total diffusion coefficient of the re-oxidation model is expressed as the following:

$$D_\beta=D_{eff}+(1/\beta)D_{Si} \quad (28)$$

This equation can be included in model 1 if D_{eff} is replaced by D_β in all the equations in model 1.

Remark 2: Because the SiO_2 of thickness y must consume the oxidated Si of thickness βy, the original location of the peak value shifts a distance of βy from the surface of the initial Si at zero to the interface of SiO_2/Si. Thus, the expression r(t) requires subtracting βy(t) during the simulation iteration process.

2.2.3.2 Description and expression for the consumption of doses in the reoxidation model

The dopants that diffuse beyond X_J', escape from the Si surface and stay in SiO_2 are all of the extra consumption of the implantation dose. This process is described in details below :

Remark 1: The first part of the consumption is the dopant dose that exceeds X_J', which does not contribute to $1/R_{\square}$.

Remark 2: The second part of the consumption is the escaped dopant dose after the thermal oxidation of t_1,

$$DS_{out}=D_{Si}\int_0^{t1}[\delta C'(x,t)/\sigma x_{x=xo(t)}]\,dt \quad (29)$$

Remark 3: The SiO_2 that is newly oxidated after duration t_1 can be handled according to the already oxidated SiO_2. Then, the issue of the dopants that escape from the SiO_2 and diffuse beyond X_J'comes down to the continuously increased standard deviations, $\sigma_{t1}'=(\sigma_{p1}^2+D_1t)^{1/2}$ in the SiO_2 direction and $\sigma_{t2}'=(\sigma_{p2}^2+D_2t)^{1/2}$ in the Si direction. This issue reflects the first and third part of the consumption of the dose, i.e. the consumption during re-oxidation and the post-high temperature $t=T_1+T_2$. Regardless of how many dopants that have escaped from SiO_2 or diffused beyond X_J, we only need to focus on the change of D_β in the SiO_2 direction and the change of $(\sigma_{p2}^2+D_2t)$ in the Si direction. If we substitute D_{eff} and σ_t in all the equations in model 1 with D_β and $\sigma_{t\beta}$ and then perform the simulation as before, the R_P/DS is obtained.

2.2.4 Model. 4: MHE T E/D S O SiO2 R O HT

Model 4 is actually a combination of model 2 and 3. The distribution parameters of model 2 are equal to the distribution parameters of the final high temperature, which are marked by"'. These parameters are the superimposition of two implantations. According to the partial differential equations in model 2, we can obtain the solutions of R_{11}''', DS_{11Si}''', R_{12}''' and DS_{12Si}'''. By using the linear superposition separation principle and gradual simulation, the suitable R_{11}, DS_{11}, R_{12} and DS_{12} are obtained. Note the first subscript, '1', denotes the distribution in Si; the second subscript '1' or '2' denotes the parameters used in the first or second implantation.

3. Discussion (Feasibility Analysis)

3.1 Verify IPQORS and Extract the Parameters by SUPREM

It is essential to fully utilize SUPREM to verify and extract model parameters. Relying on the SUPREM, IPQORS does not need to consider the LSS theoretical calculation. It thus can focus on finding feature points and distribution parameters. IPQORS can reversely simulate special distributions with quantitative implementation in one shot as well as achieve the same simulation precision as SUPREM.

3.2 Obey the Theory of Thermal Conduction and Solid Diffusion

The dopants implanted in Si under high temperatures obey thermal conduction and solid diffusion theory. Their distribution follows a normal distribution (a symmetric Gaussian distribution), which can be mathematically expressed. The implantation and diffusion of the dopants however are asymmetric. This does not interfere with the mathematical expressions and operations on the distribution mentioned above. In other words, the location of the feature point Q_2, peak value location, course dose and the standard deviation on both sides of the peak value during Dt can all be mathematically expressed.

3.3 Reverse Simulatiion of Implantation Target Parameters

For given simulation conditions, all of the processing parameters but the assistant parameter T_{OX} and C_{SUB}, are after DT e.g. X_J' and $R_{\square}$. These processing parameters, which serve as the given initial conditions of simulation, are used to develop the required implantation target parameters through iterative operations.

3.4 Obtain Implantation target parameters for the specific distribution by determining the conditional extremum of multi-variable functions

Modern deep submicron IC devices undergo the processing of low post–high temperature amount (DT_L). In the processing, the implantation distribution is the principal distribution, while the post–high temperature redistribution is supplementary. Therefore, solving the distribution parameter R_1', R_2' and DS_{2Si}' (DS_{1Si}') of the DT_L can be used for linear superposition and a separation principle under the representative DT_L, e.g. 950ºC for 20 minutes. If a post–high temperature amount greater than the DT_L is also used, it must be amended and verified by the SUPREM. Moreover, the multi-energy/dose implantation must be adopted in order to achieve a special distribution. Thus, the implantation target parameter R_1, R_2, DS_{1Si} and DS_{2Si} are obtained by solving for the conditional extremum of multi-variable functions. They are simulated using model 1.

3.5 Make Full Use of D_{eff} and σ_t

The effective diffusion coefficient and standard deviation are relevant throughout the entire course of model building. The

concept of asymmetric diffusion coefficient must be introduced because of the asymmetrical implantation distribution and the asymmetrical physical interface on both sides of the peak value location. Specifically, the diffusion coefficient in the Si direction is D_{Si} and that in the SiO_2 direction is ω (1/m) D_{Si}. The effective diffusion coefficient of the dopants in SiO_2 due to SiO_2/Si segregation thus can be expressed as ω(1/m) D_{Si}. The coefficient of the dopants that diffuse abnormally in Si is denoted as D_{eff} (D_A). Especially when Si is oxidated, it turns into SiO_2. Because of the bulk increase of 1/β times and the dopant segregation, the effective diffusion coefficient of the dopants diffusing in the SiO_2 direction is expressed as $D_\beta = [\omega(1/\beta)D_{Si}+\omega(1/m)]D_{Si}$. Based on the asymmetric diffusion, the standard deviation in the SiO_2 direction and Si direction, σ_{t1} and σ_{t2}, are also different. In order to achieve precise reverse simulation, D_β, σ_{t1} and σ_{t2} need to be fully utilized and tuned carefully. D_{eff} (D_β) and σ_t ($\sigma_{t\beta}$) are not only important feature parameters but also core model parameters.

3.6 Tests and Verification of Important Models

Model 2 is used here as an example for discussion. Equation 30, 31 and 32 are solutions of the partial differential equation 24, 25, 26 and 27

$$R'_2+2B\,R'^2_1\,R'_2-R'_1-2D\,R'^2_2\,R'_1=0 \quad (30)$$

$$f(R'_1)=2AB\exp(B\,R'^2_1)\,R'_1\,R'_2+C\exp(D\,R'^2_2)-A\exp(B\,R'^2_1)-2A\,D\exp(B\,R'^2_1)\,R'^2_2 \quad (31)$$

$$A\,DS\exp(B\,R'^2_1)-C\text{ sub-}A\exp(B\,R'^2_1)\,DS_2+C\exp(DR'^2_2)\,DS_2=0 \quad (32)$$

A, B, C, and D are the parameters that contain the standard deviations Φ'_1 (relative to R'_1) and Φ'_2 (relative to R'_2). The initial value can be determined by quasi–experience and the corresponding boundary conditions. As shown in Figure 4. F (R'_1) is a function that has an independent variable R'_1. R'_1 can be determined preliminarily according to the fact that the function f(R'_1) approaches "0" infinitely. R'_1 is selected as a value adjacent to the maximum concentration gradient at X_J. R'_2 and DS_2 are deduced from the selected R'_1, which meets the requirements of either a larger concentration gradient or a high level of smoothness. Figure 5. Shows three curves of the three corresponding group data, R'_1, R'_2 and DS_2 (DS_1), which are deduced from equation 30, 31 and 32. The given processing conditions are:

- ·Substrate N (100) 1.0E14cm^{-3}, mat SiO_2 thickness: 0.002μm
- B^+ implantation DS: 6E12cm^{-2}
- DT: 950 ºC for 10 minutes

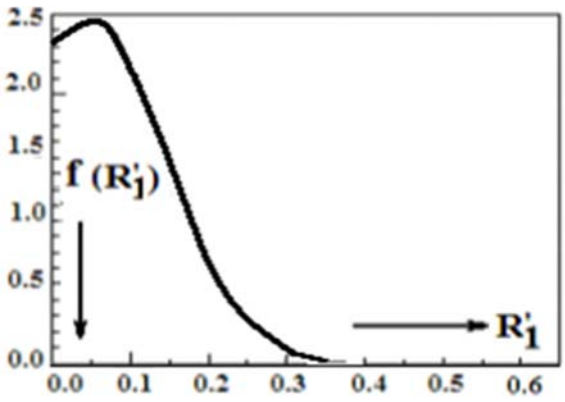

Fig 4: Plot of the Model 2equations numerical solution.

The dot-lineation shows the largest concentration gradient at the X_J with less smoothness, which fits the PN junction doping. The solid line shows a larger concentration gradient at X_J (or at the interface of the material structure modification) with more smoothness, which fits the quasi-rectanglized distribution for the material structure modification. The dashed line shows the lowest concentration gradient at X_J and the worst unknit, which is similar to a single energy/dose implantation due to the excessively large DS_2 value.

4. Conclusion

The traditional forward simulation like SUPREM has inherent weakness. It is difficult to perform a reverse simulation the target parameters in quantitative for multi-physical parameter controlling with a quasi-normal distribution.

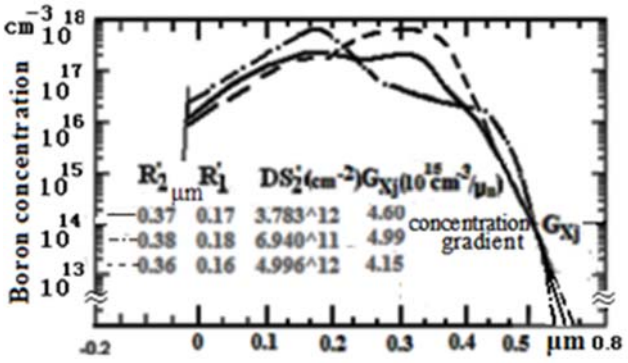

Fig 5: The curves of three corresponding groups of data, substrate N (100) 1.0E14cm-3, Mat SiO2 thick: 0.002μm;B^+ implantation DS:6E12cm^{-2} ; DT:950 ºC for 10 minutes.

The difficulties come not only from the controlling problem of multiple physical parameters, but also from the quantitative one-shot. i. e. being one-shot, multi-physical parameter and with quantitative. IPRORS, which is a one-shot simulation for a multi-physical parameter controlling with a quasi-normal distribution, can solve the problem. Although the database of IPRORS and the application software have not been developed completely, the feasibility has been fully demonstrated. The test results shown in Figure 4 and Figure 5 have proven the correctness of IPQORS. We believe IPQORS will replace SUPREM in the future once it is implemented in application software. Furthermore, the concept of reverse simulation introduced by IPRORS can be applied to other science and technology areas, especially the target parameters simulation of the multi-physical parameters controlling of a normal or quasi-normal distribution.

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