A Systematic and Physically Based Method of Extracting a Unified Parameter Set for a Point-Defect Diffusion Model

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Abstract

A systematic and physically based method for extracting of a unified parameter set for a point-defect diffusion model is proposed. A sensitivity matrix analysis is used to construct the sequence of the extraction and to select the data set to be fitted.

1. Introduction

The point-defect pair diffusion model is widely used for highly accurate process simulations, but it has been difficult to extract the parameters that can make it useful for various process conditions. Since a state-of-the-art model is based on some approximations and/or assumptions, perfect matching of the simulation results with the experiments can never be expected. Therefore, some compromise must be made. However, what to or how to compromise must be determined as objectively as possible and the compromise must be physically sound. Extracting all parameters at one time by using a least-square method or a design of experiment is not appropriate, because reduction of the global error norm does not guarantee that the obtained parameters are physically reasonable. This paper proposed a systematic and physically based method for extracting of a unified parameter set for a point-defect diffusion model for boron(B), phosphorus(P), and arsenic(As).

2. General rule of parameter extraction

To make a systematic and physically based extraction possible, we introduced the following general rules.

The first rule is that the parameters are extracted one by one so that the simulation results should agree with the measured 1D profiles. However, in the case that some parameters have a strong correlation with one other, they are determined simultaneously.

The second rule is that the order of the extraction and the process conditions to be used at each extraction step are determined so that the process conditions should be sensitive to the focused parameters but less sensitive to the parameters not yet determined (= lower priority parameters). This task is made easier by constructing matrices of sensitivity for parameters and process conditions. As an example, a parameter sensitivity matrix for implanted ion and dose is shown in Table 1. The

parameters are listed according to the order of the extraction and the process conditions used in each extraction step are marked with a double underline.
The third rule is that the higher priority parameters are re-adjusted if a satisfactory agreement with the measured profile cannot be obtained by adjusting the lower priority parameters.

Table 1: Matrix of sensitivity for parameters and process conditions.

Parameter	Impurity/Dose			Ex.)
	B	P	As	
	L ↔ H	L ↔ H	L ↔ H	Fig.
$K_{\rm I}^{srf}$	$\underline{\underline{◎}}$ ◎ ○	$\underline{\underline{◎}}$ ◎ ○	○ ○ ○	2
$k_{\{311\}}$, $K_{\{311\}}^{eq}$	△ ○ ○	○ $\underline{\underline{◎}}$ ◎	× ○ ○	3
$K_{\rm I}^{sink}$	× ○ ○	× ○ $\underline{\underline{◎}}$	× × ○	4
B cluster	× $\underline{\underline{○}}$ $\underline{\underline{◎}}$	-	-	5
As cluster, $E_{\rm AsI}^{bin}$, $E_{\rm AsV}^{bin}$, $f_{\rm AsI}$	-	-	× $\underline{\underline{○}}$ $\underline{\underline{◎}}$	6

◎ ○ △ × : Sensitivity for parameter
$\underline{\underline{◎}}$ $\underline{\underline{○}}$: Selected conditions for extraction

3. Parameter extraction

A parameter extraction method for the previously proposed point-defect pair diffusion model [1] was constructed based on the general rules. The procedure is shown in Fig. 1. The model parameters were classified into four categories.

First, the most fundamental parameters are determined. Since these parameters are sensitive to the simulation results, thier values have to be determined first. Unfortunately, some of these values can not be measured by experiments. Therefore, the values in the literatures [2]-[6] are used as initial values and then later are re-adjusted according to the feedback from the lower priority parameters.

Second, the parameters related to pair reactions are determined. From these parameters, $k_{\rm B/I}$, ..., $K_{\rm BI}^{eq}$, ..., and $D_{\rm BI}$, ... are *automatically determined* (see Table 2). An accurate extraction is not necessary at this step, because their values are less sensitive to the degree of transient enhanced diffusion (TED). $f_{\rm PI}^{0}$ and $f_{\rm PI}^{-}$ are provisionally determined as 1 at this step and are revised later. The parameters for As are also determined later with the parameters for As cluster.

Next, the parameters related to point-defects are extracted. They are responsible for the simulation being accurate because they directly control the life time of interstitial after ion implantation. The sequence of the extraction and the selection of the process conditions to be used are therefore very important. The extraction sequence was determined according to the second general rule. The actual sequence is as follows: 1. The value of $K_{\rm I}^{srf}$ was determined using the profiles measured after low dose B or P implantation and annealing until TED finished (Fig. 2). 2. The values of $k_{\{311\}}$ and $K_{\{311\}}^{eq}$ were determined using the profiles measured after middle dose P implantation and rapid annealing at a low temperature (Fig. 3). 3. The point-defect sink term $K_{\rm I}^{sink}$ which is related to ion implantation damage was determined using the profiles measured after middle-high dose P implantation and annealing (Fig. 4).

Finally, the parameters related to each impurity clustering are determined. They are responsible for diffusion after high dose ion implantation. It is possible to extract parameters for each impurity independently. In our diffusion model [1], the parameter values for B and As clustering were extracted (Fig. 5, 6). Regarding As, the samples which include B are adopted as well, because the coexistent B can be used as a marker for the degree of interstitial generation. The values of $E_{\rm AsI}^{bin}$, $E_{\rm AsV}^{bin}$, and $f_{\rm AsI}$ in the second category are extracted simultaneously.

4. Verification

Electrical characteristics of actual devices were calculated by using a 2D process simulator with the extracted model parameters, and then their measurements were compared. The measured and simulated $V_{th} - L_{gate}$ characteristics of the 0.35μm, 0.25μm, and 0.18μm generation MOSFETs are shown as examples in Fig. 7-9. The simulated results reproduce the short channel effect of p-MOS and the reverse short channel effect of n-MOS.

Table 2: Symbols of parameters.

Parameter	Symbol
Diffusion constant of X	D_X
Intrinsic diffusion constant of X	D_X^{intr}
Equilibrium concentration of X	C_X^*
Energy level of charged X	e_X
Barrier-energy of X/Y reaction	$\Delta E_{X/Y}$
Binding-energy of XYpair	E_{XY}^{bin}
Factor of I mechanism of X	$f_{X\mathrm{I}}$
Generation rate of X	k_X
Resolution rate of X	k_X/K_X^{eq}
Surface recombination rate of X	K_X^{srf}
Absorption rate of X in sink term	K_X^{sink}
$k_{X/Y} = 4\pi r\cdot(D_X+D_Y)\cdot\exp(-\Delta E_{X/Y}/k_BT)$	
$K_{XY}^{eq} = 4/C_{Si}\cdot\exp(E_{XY}^{bin}/k_BT)$	
$D_{X\mathrm{I}} = f_{X\mathrm{I}}\cdot D_X^{intr}/C_\mathrm{I}^*/K_{X\mathrm{I}}^{eq}$	
$D_{X\mathrm{V}} = (1-f_{X\mathrm{I}})\cdot D_X^{intr}/C_\mathrm{V}^*/K_{X\mathrm{V}}^{eq}$	

5. Conclusion

A systematic and physically based method for extracting a unified parameter set for a B, P, As, and point-defect pair diffusion model has been proposed. A sensitivity matrix is used to construct the sequence of the extraction and to select the data set to be fitted at each step. The parameters are classified into four categories according to their extraction priorities.

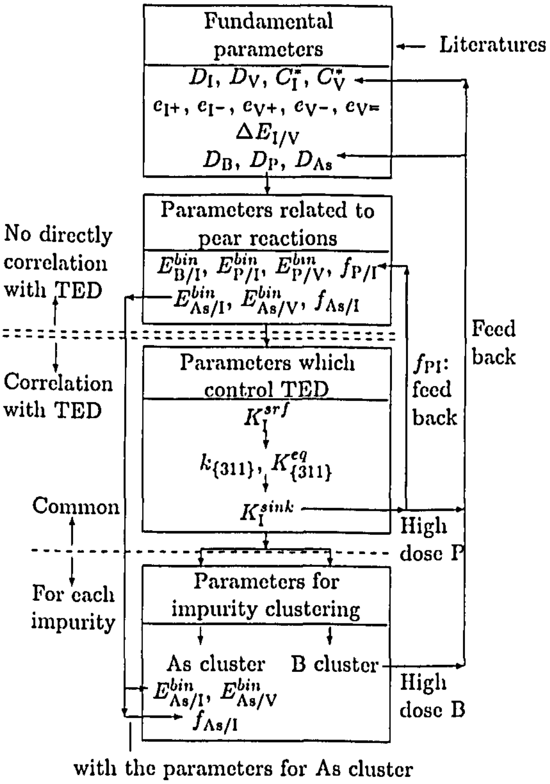

Figure 1: Flow of the extraction.

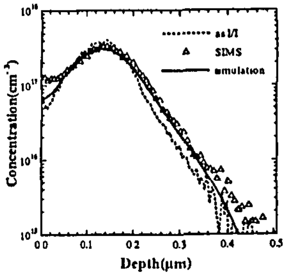

Figure 2: B 40keV 5 × 10^{12} cm^{-2} implantation followed by 1125°C 10 sec RTA.

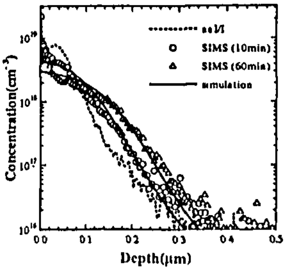

Figure 3: P 40keV 5 × 10^{13} cm^{-2} implantation followed by 750°C 10 min /60 min anneal.

It is shown that the extracted unified parameter can be applicable to various process conditions.

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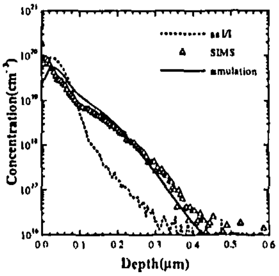

Figure 4: P 40keV 5×10^{14} cm^{-2} implantation followed by 850°C 10 min anneal.

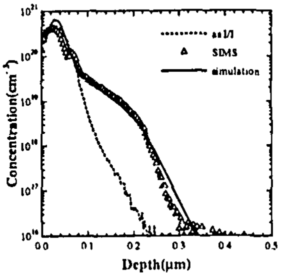

Figure 5: BF$_2$ 50keV 3×10^{15} cm^{-2} implantation followed by 850°C 60 min anneal.

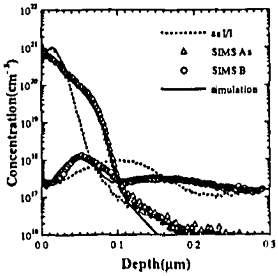

Figure 6: B 30keV 1×10^{13} cm^{-2} + As 30keV 3×10^{15} cm^{-2} implantation followed by 850°C 60 min anneal.

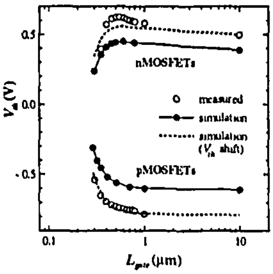

Figure 7: $V_{th}-L_{gate}$ characteristics of the 0.35μm generation MOSFETs.

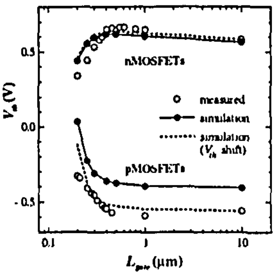

Figure 8: $V_{th}-L_{gate}$ characteristics of the 0.25μm generation MOSFETs.

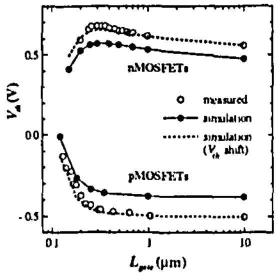

Figure 9: $V_{th}-L_{gate}$ characteristics of the 0.18μm generation MOSFETs.