Methodology for Prediction of Ultra Shallow Junction Resistivities Considering Uncertainties with a Genetic Algorithm Optimization

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ABSTRACT

The accurate prediction of arsenic activation after spike annealing is mandatory for Ultra Shallow Junction (USJ) sheet resistance optimization for advanced NMOS transistors engineering. For the first time, we propose a fast and efficient methodology which consists in both predicting coefficients which model the arsenic activation, and in calibrating a physically-based mobility model from experimental data. Calibration was obtained by a genetic algorithm optimization of a criterion taking into account the difference between simulation and measurement, and both experimental and modelling uncertainties.

Keywords: arsenic activation, modelling, calibration, DoE, optimization, genetic algorithm, analysis of variance

1 INTRODUCTION

As device downscaling continues, the sheet resistance of source/drain diffusion areas (S/D) becomes the major limiting factor of the deep submicron device performance [1]. To obtain low resistance USJ as required for nanoscale devices, spike anneals are usually performed. These anneals (a few seconds at 1050°C) allow to achieve high doping level activation with little diffusion. In the case of arsenic it is known that for high doping concentration, a fraction of dopants remains electrically inactive after the anneal. It is accepted that the inactive unprecipitated dopant is in a clustered form, in a mass action equilibrium with the ionized As [2]. The rigorous prediction of inactive fraction would require dynamic models that describe the formation and the kinetic evolution of each population of a great number of different arsenic-vacancies defects. However, such a model has not been reported in literature until now.

In this work, we propose a new methodology to determine, from an empirical modelling, the electrically active arsenic distribution after a 1050°C spike anneal for a wide range of ion implantation conditions.

2 EXPERIMENTAL DATA

In order to ensure the statistical confidence on the results, experiments have been performed following two adjacent standard 3^2 Design of Experiments (DoE) on the two implantation factors : energy and dose. The center of each design was replicated 3 times on different wafers to estimate the experimental dispersion. 8" P-type substrates were implanted with arsenic through a 2 nm screen oxide, with an EATON NV8200P implanter. The details of the ion implantation conditions are given in table 1. Finally dopants activation was performed with a 1050°C spike annealing.

	Energy (keV)	Dose (cm^{-2})	Rsheet measured values (Ω/□)	σ (%)	Rsheet optimized values (Ω/□)
P1	3	10^{13}	14500	14	14214
P2	3	$2.5\ 10^{14}$	1120	9.1	1091
P3	3	$5\ 10^{14}$	750	4.7	749
P4	3	$1.75\ 10^{15}$	320	4	333
P5	3	$3\ 10^{15}$	290	5.2	289
P6	9	10^{13}	5700	12.5	5423
P7	9	$2.5\ 10^{14}$	555	4.5	546
P8	9	$2.5\ 10^{14}$	580	5.2	583
P9	9	$2.5\ 10^{14}$	545	4.6	541
P10	9	$2.5\ 10^{14}$	560	3.6	577
P11	9	$5\ 10^{14}$	374	4	385
P12	9	$1.75\ 10^{15}$	220	4.6	225
P13	9	$1.75\ 10^{15}$	220	3.2	218
P14	9	$1.75\ 10^{15}$	205	6	200
P15	9	$1.75\ 10^{15}$	218	3.7	212
P16	9	$3\ 10^{15}$	193	3.6	185
P17	15	10^{13}	4500	6.7	4557
P18	15	$2.5\ 10^{14}$	430	4.7	417
P19	15	$5\ 10^{14}$	273	4.5	267
P20	15	$1.75\ 10^{15}$	161	4.3	162
P21	15	$3\ 10^{15}$	152	3.8	159

Table 1: Experimental ranges for arsenic implantation following two adjacent standard 3^2 DoE, R_{sheet} measurements with its standard deviation σ, and R_{sheet} values predicted after the optimization stage.

The As chemical profile is obtained from SIMS measurements. The MCs_2^+ technique was used [3] on a Cameca IMS-5f instrument with a primary (Cs^+ beam) impact energy and incidence angle of 1 keV and 50° respectively, in order to reduce ion beam mixing and equilibration depths.

Four-point probe measurements were also performed to get the sheet resistance (see table 1).

3 ELECTRICAL RESPONSE MODELLING

To determine the As active distribution we adopted an inverse modelling methodology. Actually we look for the profile which modelled R_{sheet} value is as close as possible to the corresponding experimental value.

The sheet resistance is modelled by :

$$R_{sheet} = \left(\int q \, N_{active}(x) \, \mu(N_{active}(x), N_{inactive}(x)) dx \right)^{-1} \quad (1)$$

$N_{active}(x)$ and $N_{inactive}(x)$ are the active and inactive arsenic distributions respectively. μ is the mobility model as explained in section 3.2.

3.1 Active arsenic distribution

The active arsenic profile $N_{active}(x)$ is obtained by truncating the chemical profile $C_{As}(x)$ at a maximum concentration value C_lim representing the electrical solubility threshold of arsenic into silicon. C_lim is usually set to 2×10^{20} cm^{-3} [2].

As the calculation of R_{sheet} with a constant C_lim leads to big discrepancies with the experimental values (see "Literature data" in figure 5), we have improved the modelling of the active profile. Indeed, on the one hand we assumed that C_lim is a function of the implantation conditions, and on the other hand the As active distribution is assumed to have a constant drop at the interface SiO_2/Si due to pile-up (figure 1).

$$N_{active}(x) = \frac{x}{C_1} C\_lim \quad \text{for } x < C_1 \quad (2)$$

where C_1 is the characteristic length of the pile-up decay.

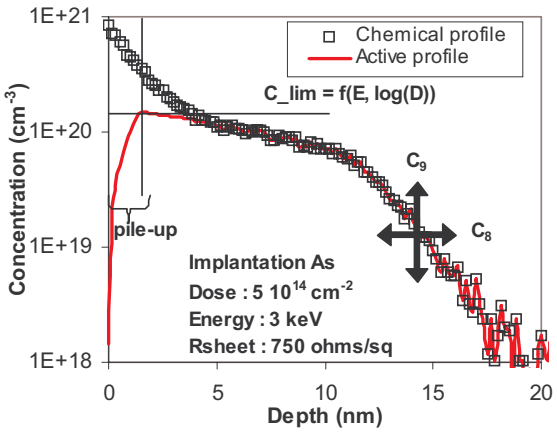

Figure 1: Example of the chemical and active As profile obtained after optimization

Then C_lim was extracted for each experiment of the DoE while keeping the mobility model parameters to their literature value.

Finally a quadratic model of the response log(C_lim) as a function of the factors log(dose) and energy was generated with the software ECHIP [4].

$$\log(C\_lim) = C_2 + C_3 \log(dose) + C_4 \log(dose) \cdot energy + C_5 (\log(dose))^2 + C_6 \, energy^2 \quad (3)$$

The linear term in energy of that empirical model has been removed since its effect is negligible according to the Pareto effects graph in figure 2.

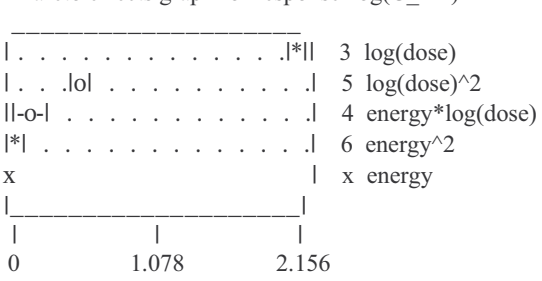

Figure 2: Pareto effects graph giving the classified effects of the factors scaled to units of the response log(C_lim), with their confidence intervals.

With an adjusted R^2 of 0.99, the quality of the RSM model is very satisfactory. Moreover figure 2 shows small confidence intervals, then the accuracy of the terms of the model may be quite good. The coefficients generated by ECHIP are displayed in table 2.

In figure 5 we compare results obtained with literature data, and those using the empirical model of C_lim and including the pile-up effect (called "First fit"). It appears that the new modelling of the active profile gives better predicted R_{sheet} values than before.

3.2 Mobility model

The mobility model μ from (1) is a Mathiessen's combination of two mobility models μ_{active} and $\mu_{inactive}$ depending on the active and inactive As profile respectively.

$$\frac{1}{\mu} = \frac{1}{\mu_{active}} + \frac{1}{\mu_{inactive}} \quad (4)$$

μ_{active} corresponds to the Masetti's model with parameters set to their initial value [5].

$$\mu_{active} = \mu_0 + \frac{\mu_{max} - \mu_0}{1 + \left(\frac{N_{active}(x)}{C_r} \right)^{\alpha}} - \frac{\mu_1}{1 + \left(\frac{C_s}{N_{active}(x)} \right)^{\beta}} \quad (5)$$

$\mu_{inactive}$ is a term added by Rousseau et al. [6] to take into account carrier interaction with neutral inactive defects.

$$\mu_{inactive} = \frac{K\,q}{m^* N_{inactive}(x)} \quad (6)$$

where q is electron charge, m* is its effective mass (we used m*=0.26 of electron mass). K is the Rousseau's fitting parameter for neutral scattering ($K=4.59\times10^7$ $cm^{-3}s$).

4 OPTIMIZATION CONSIDERING UNCERTAINTIES

To determine more rigorously the value of the parameters of (1) and particularly those used to obtain $N_{active}(x)$, we have to choose a criterion to be minimized. According to the Maximum Likelihood theory [7], the most probable parameters should minimize the following expression :

$$S = \sum_{j=1}^{21} \frac{\left(h_{measured\ j} - h_{predicted\ j}(C_1, ..., C_{13}) \right)^2}{\sigma_j^2 + \sum_{i=1}^{13} \left(\frac{\partial h_{predicted\ j}(C_1, ..., C_{13})}{\partial C_i} \right)^2 . \sigma_{C_i}^{\ 2}} \quad (7)$$

where $h=R_{sheet}^{-1}$ is a transformation which linearize S to make the numerical optimization easier.

The parameters C_1, ..., C_{13} are to be optimized and their initial value is given in table 2. C_1 corresponds to the characteristic length of the pile-up drop. C_2, ..., C_6 correspond to the coefficients of the quadratic model (3). C_7 is a parameter that makes the transition between the chemical profile and C_lim smooth. The SIMS error on the profile depth and the concentration [3] are also taken into account with parameters C_8 and C_9 respectively. Their values are close to the unity.

$$C_{As}(x, C_8, C_9) = C_9 . SIMS(C_8 . x) \quad (8)$$

where SIMS(x) is the experimental chemical profile of arsenic.

Finally C_{10}, ..., C_{13} are the mobility parameters μ_1, β, Cs and K chosen to be optimized as done in [6].

The coefficient σ_j in the expression (7) is the standard deviation of each R_{sheet}^{-1} measurement. σ_{Ci} is the standard deviation of each model parameter obtained from analysis of results given by ECHIP for the coefficients of the quadratic model (3) and from literature data ([2], [3], [5] and [6]) for the other parameters. The search range of the parameters is taken to the nominal value ± σ_{Ci}.

	Lit. data value	**First fit**	**FEP optim.**
C_1 (nm) Є [0.1,3]	–	1.5	1.4
C_2 Є [19,21]	20.3	19.6945	19.655
C_3 Є [0.8,0.9]	–	0.85	0.89
C_4 Є [-0.0081,-0.0075]	–	-0.0791	-0.00786
C_5 Є [-0.4,-0.3]	–	-0.3561	-0.4
C_6 Є [0.0006,0.00064]	–	0.000625	0.00061
C_7 Є [0.7,0.99]	–	0.9	0.76
C_8 Є [0.975,1.025]	1	1	0.975
C_9 Є [0.95,1.05]	1	1	0.95
$C_{10}=\mu_1$ (cm^2/Vs) Є [30,50]	43.4	43.4	36.4
$C_{11}=\beta$ Є [1.8,3]	2	2	3
$C_{12}=Cs$ (cm^{-3}) Є [2.5-4 10^{20}]	3.43 10^{20}	3.43 10^{20}	2.61 10^{20}
$C_{13}=K$ ($cm^{-3}s$) Є [3-6 10^7]	4.59 10^7	4.59 10^7	3 10^7
S	**178**	**16.5**	**6.8**

Table 2: R_{sheet} model parameters before and after optimization, with their search range estimated from the confidence intervals of the Pareto effects graph (Figure 2).

Facing this high dimensional (13 parameters) optimization task, we have implemented in the software MATHCAD [8] a Fast Evolutionnary Program (FEP) based on Yao work [9]. This global optimization method is a particular case of Genetic Algorithms, known to find the global optimum in most cases without getting trapped by local minima. The flowchart of the algorithm used is detailed in figure 3.

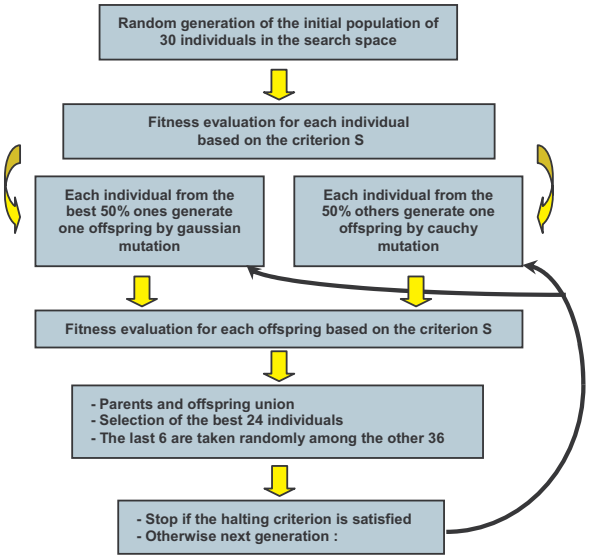

Figure 3: Flowchart of the Evolutionnary Programming algorithm used in the parameters optimization

5 RESULTS

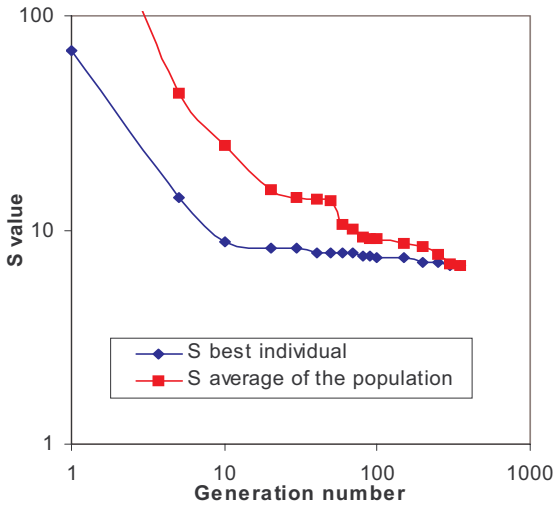

Figure 4: Convergence of the FEP.

Figure 4 shows the evolution of the value of the S criterion when the number of generations is increased. It indicates that after 350 generations, the algorithm has probably converged on the global minimum since most individuals of the population are very close to the best individual. In addition the best individual of the population changes only a little after the generation 100.

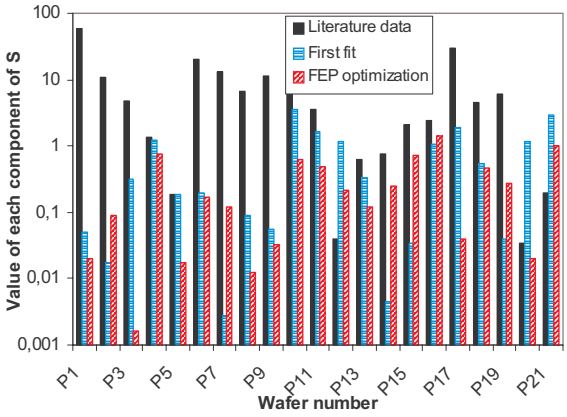

Figure 5: Comparison of each component value of the S criterion obtained with literature data parameters, with values from the empirical model of C_lim and considering pile-up effect, and with parameters given by the genetic optimization.

The values of the thirteen parameters obtained after the genetic optimization are given in table 2. One can see that the optimized set of coefficients gives the lowest criterion value of the three trials. The values of R_{sheet} predicted by (1) after the FEP optimization are displayed in table 1. These values are quite close to the experimental ones. Indeed figure 5 shows that the components of the S criterion have been, on the whole, improved after the FEP optimization compared with previous work.

6 CONCLUSION

An efficient and statistically rigorous methodology has been developped to calibrate a high number of model parameters required to simulate the USJ resistivity. The method accurately predicts the arsenic active distribution for a wide range of ion implantation conditions and a 1050°C spike anneal. The method also optimizes, with a genetic algorithm, the relevant set of model parameters, considering the experimental and modelling uncertainties.

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