Predictive and Calibrated Simulation of Doping Profiles: Low Energy As, B and BF_2 Ion Implantation

P. Scheiblin, F. Roger*, D. Poncet, C. Laviron, P. Holliger, F. Laugier, E. Guichard*, J.P. Caire**.

LETI (CEA-Grenoble), 17, rue des Martyrs, 38054 Grenoble Cedex 09, France, pscheiblin@cea.fr
*SILVACO Data Systems, 8 avenue de Vignate, Actimart de Gières, 38610 Gières, France, frederic.roger@silvaco.com
** LEPMI-ENSEEG, 1130 rue de la Piscine, BP 75, 38402 St Martin d'Hères cedex, France, jean-pierre.caire@inpg.fr

ABSTRACT

In this work, we propose calibrated models for predictive simulation of low energy Arsenic, Boron and BF_2 ion implantation in the suitable range for sub-100nm CMOS technology.

The International Technology Roadmap for Semiconductors (ed. 1999) underlines the need for development of analytical models for ion implantation simulations, supported by Monte Carlo models. These models become more and more complex, from the simple Gaussian approximations to the latest double Pearson-4 distributions, or Legendre polynomials fitting.

Leaving apart the domain of the sophisticated ion implantation models, we found that the value of the doping concentration itself could be expressed with a fair accuracy, as a function of the experimental conditions. The predictivity of this technique is insured by the use of Design Of Experiments and Response Surface Methodology.

Keywords: Calibration, TCAD, Ion Implantation, DoE, RSM.

1 INTRODUCTION

The predictive calibration of the parameters of modern models for ion implantation such as dual Pearson-4 distributions (DP4) [1] or Legendre polynomials (LP) [2] is a critical task. The main reason is the large number of difficult-to-extract parameters of model, compared with the low number of available experiments.

However, using a calibration methodology [3] based on Design of Experiments (DoE) and Response Surface Methodology (RSM), we found an efficient technique to predict any implant of low (3-10 keV) energy Boron, BF_2 and Arsenic ions, varying dose and energy.

2 NEW APPROACH FOR MODELING PROFILES

In standard implantation modeling (DP4 or LP), the concentration is a function of depth, whose coefficients are stored in lookup tables, for different experimental conditions. Thus, a large number of experiments is required to get a profile by linear interpolation. Moreover, there are no confidence limits on the predictions.

We have already addressed the question of calibration of LP [4]. Here, however, we will model the implanted profiles following a very simple methodology, called Sampling CALibration of Profiles (SCALP):

- first, implantation experiments are performed according to a DoE ;
- then, the SIMS doping profiles are normalized in depth with respect to the total profile extent (where concentration falls below 10^{18} cm^{-3}, for example);
- next the concentrations are extracted at given percentages of the total depth ;
- finally concentrations and total depth are expressed by RSM polynomials, as functions of the process factors.

Thus, this single set of polynomials allows an easy calibrated modeling of any new implantation profile (see figure 1). For a sampling of the concentration every 5% of the total depth, 20 polynomials allow the modeling of any implantation profile.

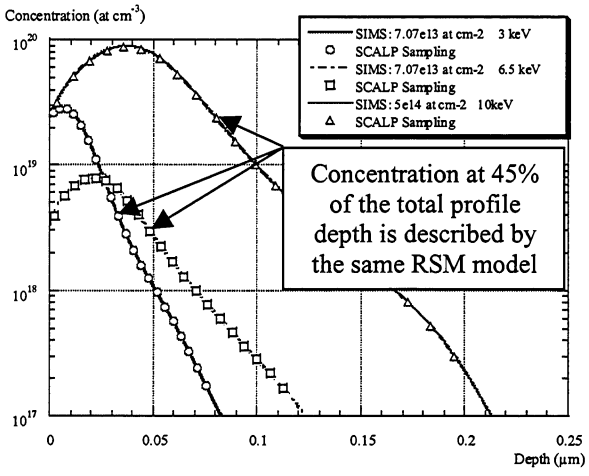

Figure 1: Illustration of the SCALP technique: the concentration at a given percentage of the total depth follows the same quadratic polynomial model, which is a function of the process factors dose and energy.

The use of DoE minimizes the number of experiments and gives a statistical significance to the predictions of the calibrated implantation model. An other advantage of the method is that it implicitly takes the dose loss into account.

This approach can be extended to other process parameters like tilt, twist or screen oxide thickness.

3 EXPERIMENTAL

A standard 3^2 DoE is used in the aim of obtaining a quadratic modeling of the responses depth and log(concentration), as a function of the factors log(dose) and energy:

$$\log(conc) = \beta_0 + \beta_1 \log(dose) + \beta_2 energy + \beta_3 \log(dose) \cdot energy + \beta_4 (\log(dose))^2 + \beta_5 energy^2$$

The center of the design is replicated 3 times on different wafers to estimate the experimental dispersion.

The experimental ranges are given in table 1 :

	Energy (keV)	Dose (cm^{-3})	Tilt (°)	Twist (°)
Arsenic	3 - 10	$3\ 10^{13}$ to 10^{15}	7	27
Boron		10^{13} to $5\ 10^{14}$		
BF_2		$3\ 10^{13}$ to 10^{15}		

Table 1: Experimental ranges for Arsenic, BF_2, Boron.

The implantations were performed on 8" Si wafers, through a 2 nm screen oxide, with an EATON NV8200P implanter. The characteristics of the energy filter of this equipment allow a high purity of the beam, leading to very good repeatability of the experiments.

The analysis of these narrow profiles requires carrying out a specific measurement technique [5]: SIMS measurements were performed using a CAMECA IMS-5f with an effective impact energy and incidence angle of 1keV and 60° respectively, in order to reduce ion beam mixing and equilibration depths.

4 RESULTS

The total profile depth was defined for $C_{TotalDepth}=10^{17}$ cm^{-3} for Boron and BF_2, and $C_{TotalDepth}=10^{18}$ cm^{-3} for Arsenic, regarding to the noise level of the particular SIMS technique, which is higher than with standard analysis energies.

The empirical models of the concentrations and depth were generated with the software ECHIP [6]. For each of the three dopants, the quality of the RSM models is very satisfactory: the adjusted R^2 is higher than 0.8 for the major part of the profile for Boron and BF_2, as shown in figure 2. In the case of Arsenic, the very abrupt shape of the SIMS profiles entails a lack of accuracy in the tail of the curve, above 60% of the total depth.

The Pareto graphs in figure 3 show a fair precision in the classification of the effects of the factors on two responses: depth and concentration at 30% depth for Boron.

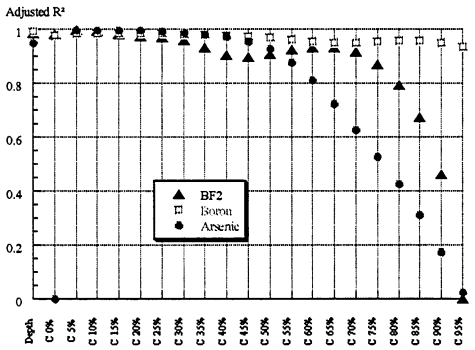

Figure 2: The values of the adjusted R^2 higher than 0.8 indicate the quality of the RSM, particularly in the case of Boron and BF_2.

The coefficients of the quadratic models are given for the total depth and some concentrations in tables 2-3-4 respectively for B, BF_2 and Arsenic. They allow the prediction of any profile within the experimental range.

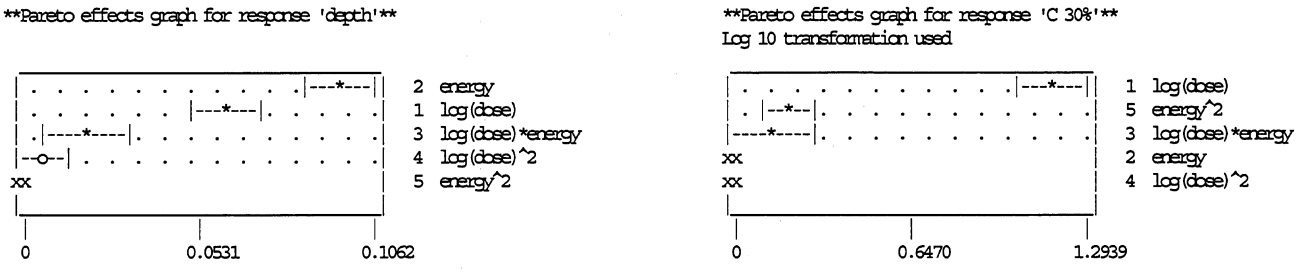

Figure 3: Pareto effect graphs giving the classified effects of the factors on the responses with their confidence intervals, in the case of Boron.

Furthermore, and unlike the "manual" tuning of analytical implantation, the simulations are predictive within a 95% confidence interval. Inside this interval, in the case of Boron, log(concentration) is predicted at +/-2% and depth at +/-10%.

	Constant	log(d)	W	log(d)*W	log(d)²	W²
Depth	1.28E-01	3.60E-02	1.39E-02	3.15E-03	-8.30E-03	2.52E-04
C 0%	1.86E+01	8.53E-01	-1.14E-01	-1.13E-02	1.47E-01	3.25E-02
C 10%	1.89E+01	9.70E-01	-6.64E-02	8.27E-03	2.60E-02	2.65E-02
C 20%	1.89E+01	8.43E-01	-2.20E-02	2.57E-02	3.46E-02	2.03E-02
C 30%	1.88E+01	6.87E-01	6.69E-03	2.67E-02	4.64E-02	1.60E-02
C 40%	1.85E+01	5.43E-01	1.48E-02	1.42E-02	8.26E-02	1.35E-02
C 50%	1.82E+01	4.41E-01	1.25E-02	5.42E-03	1.03E-01	1.20E-02
C 75%	1.76E+01	3.27E-01	4.96E-03	2.06E-03	1.05E-01	8.71E-03

Table 2: Boron case; centered variables; "d"=dose; "W"=energy.

	Constant	log(d)	W	log(d)*W	log(d)²	W²
Depth	5.97E-02	1.99E-02	5.57E-03	1.07E-03	-2.46E-03	-1.01E-04
C 0%	2.01E+01	1.09E+00	-4.90E-02	-8.22E-03	4.38E-01	-4.65E-03
C 10%	2.01E+01	8.13E-01	1.17E-02	3.50E-02	-1.77E-01	-1.47E-03
C 20%	1.94E+01	5.27E-01	2.86E-02	3.78E-02	-6.34E-03	5.34E-03
C 30%	1.88E+01	2.87E-01	2.55E-02	2.58E-02	4.87E-02	3.16E-03
C 40%	1.84E+01	1.56E-01	2.96E-02	2.26E-02	-2.20E-02	3.45E-04
C 50%	1.82E+01	1.00E-01	3.44E-02	2.13E-02	-9.18E-02	-1.03E-03
C 75%	1.76E+01	3.86E-02	2.58E-02	4.65E-03	-6.58E-02	-2.04E-03

Table 3: BF_2 case; centered variables; "d"=dose; "W"=energy.

	Constant	log(d)	W	log(d)*W	log(d)²	W²
Depth	2.42E-02	5.36E-03	2.16E-03	1.61E-05	1.46E-04	-4.81E-05
C 5%	2.00E+01	1.07E+00	-1.37E-01	1.79E-02	9.52E-02	1.12E-02
C 10%	2.01E+01	1.01E+00	-1.02E-01	1.27E-02	-5.89E-02	1.19E-02
C 20%	2.02E+01	9.31E-01	-4.41E-02	2.17E-02	-8.25E-02	1.40E-03
C 30%	2.02E+01	8.26E-01	1.28E-03	4.00E-02	-1.05E-01	-8.64E-03
C 40%	2.00E+01	6.71E-01	2.88E-02	5.89E-02	-2.05E-01	-1.14E-02
C 50%	1.96E+01	4.90E-01	3.49E-02	6.63E-02	-2.39E-01	-9.76E-03
C 75%	1.87E+01	1.28E-01	1.42E-02	3.20E-02	-1.64E-01	-1.59E-03

Table 4: Arsenic case; centered variables; "d"=dose; "W"=energy.

The excellent predictive capability of the models is obvious in figures 4 and 5 for Boron and Arsenic respectively: the prediction of the model is superimposed with test points, which were not used to generate the model and with default simulations using the SIMS Verified Dual Pearson model of ATHENA [7] (SVDP).

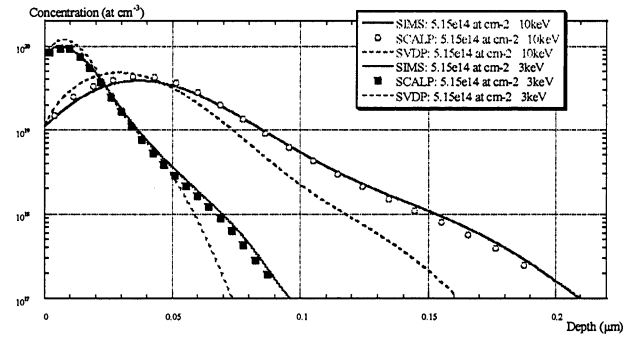

Figure 4: Calibrated predictions of Boron test points compared to SIMS and SVDP.

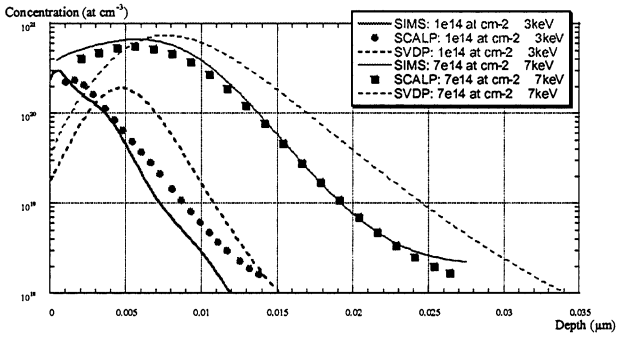

Figure 5: Calibrated predictions of Arsenic test points compared to SIMS and SVDP.

A criterion is necessary to measure the global improvement generated by our calibration technique. We choose the Root Mean Square Relative Error (RMSRE) :

$$RMSRE = \sqrt{\sum_{i=1}^{n} \frac{1}{n} \left(\frac{y_{exp_i} - y_{sim_i}}{y_{exp_i}} \right)^2}$$

where y_{expi} and y_{simi} are respectively the i^{th} experimental and simulated concentration values of a n points discretization of the profile.

In figure 6, we show the overall decrease of the RMSRE, over the whole Arsenic and Boron profile database, in comparison with simulations performed with the SVDP model. SCALP permits to divide the RMSRE average value on all the profiles, by a factor 3 for Boron and BF_2 to 8 for As.

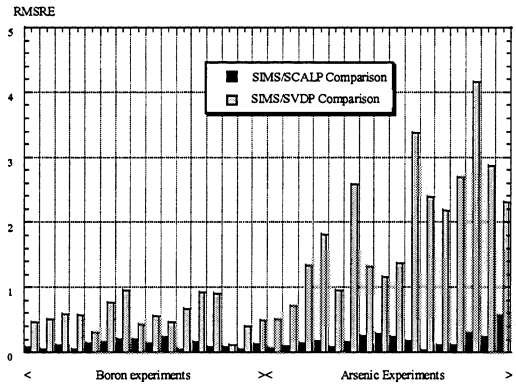

Figure 6: Graph showing the overall improvement of the RMSRE for Arsenic and B.

5 CONCLUSION

We have presented an efficient technique for predictive simulation of ion implantation. The methodology allows the calibration of Arsenic, BF_2 and Boron profiles, with the knowledge of a confidence interval, for the low energy, high dose conditions of sub-100nm CMOS technology

REFERENCES

[1] Al. F. Tash. - J. Elec. Soc. 136(3) 1989.

[2] G. Balamurugan, B. Obradovic, G. Wang, Y. Chen, Al. Tasch. - IEDM'98, p 517.

[3] G. Le Carval P. Scheiblin, D. Poncet, P. Rivallin - SISPAD'97, p 177.

[4] F. Roger, P. Scheiblin, D. Poncet, G. Le Carval, C. Laviron, P. Holliger, E. Guichard, J.P. Caire. - IWSM'2000, p 19-22.

[5] Ph. Holliger et al - Proc. of 13th An. Workshop on SIMS.

[6] ECHIP 6.4 user's guide.

[7] SILVACO International - ATHENA user's guide.