# A Method of MOSFET Dopant Profile Prediction and its Use in Transistor Design

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## ABSTRACT

As MOS transistor size shrinks to sub-quarter-micron dimensions, accurate knowledge of the dopant concentration in various regions of the transistor is becoming more and more important for device simulations. We have developed a methodology to quickly and accurately predict the dopant profiles in source/drain-extender (MDD) and pocket regions of CMOS transistors using a limited set of profile measurements. This, coupled with a method to study the effect of profile variations on transistor performance, is presented here. In the phenomenological modeling approach we propose here, we parameterize the measured profiles for a few design points carefully chosen using standard DOE techniques. The number of profile parameters is reduced by modeling the interdependencies of some of the parameters using response surface method (RSM), and determining a small subset of independent parameters. The profile parameters are then used in a two-step device design method. The first step relates process settings such as implant dose and energy to the profile parameters. In the second step, we model (using RSMs) device performances such as drive current, threshold voltage, and off current as functions of profile parameters using a tuned device simulator. This two-step modeling method helps separate the effects of process parameters from device design. The sets of models thus obtained provide a fast and accurate method of profile prediction and its use in device simulation.

**Keywords**: MOSFET, Dopant Profiles, Process Synthesis, CMOS Transistor Design.

## INTRODUCTION

In the design of CMOS transistors for VLSI technology, precise engineering of dopant profiles is very important. As the device size shrinks, accurate prediction of the extrinsic dopant profiles becomes crucial for simulating the device and predicting its performance. Predicting the performance is necessary to make decisions in the design phase. Due to these reasons, use of process and device simulators is on the rise. Common concerns in using process simulators to predict the dopant profiles in different regions of a MOSFET are accuracy of prediction, effort required to tune the simulator, computational time, etc. In the methodology we propose here, all these difficulties are reduced by employing a phenomenological approach combined with an analytical description of dopant profiles at the end of process flow.

A CMOS transistor fabrication sequence typically includes the introduction of dopants by ion implantation followed by thermal anneals. Thermal anneals are needed for several reasons such as dopant activation and implant damage removal. In some cases, thermal anneal is an unwanted effect of other processing steps such as gate oxide formation. During a transistor design process, an engineer may be required to simulate the transistor for many different implant conditions. Typically, the anneal sequence is fixed for all these conditions. Most process simulators predict the as-implanted dopant profile and redistribute it using physical models for the effect of thermal anneals. This adds computational time and complexity to the profile prediction at the end of the process sequence. Also, nowadays more and more furnace anneals are being replaced by rapid thermal anneal (RTA). Most process simulators show reduced accuracy in modeling dopant diffusion during RTA steps due to complex physical phenomena occurring in transient conditions.

One typical example of a complex diffusion mechanism during RTA is the region under the gate edge in an NMOS transistor with pocket (halo) implant. The moderately doped (MDD) region is realized by implanting arsenic, while the pocket is obtained by implanting boron. These two implants are done in succession and are followed by RTA. During this RTA, the implant damage caused by arsenic affects the diffusion of boron. Hence the final profile of boron depends on both boron as well as arsenic implant conditions.

As-implanted profiles have been modeled by Crandle, *et al.* [1] and Tasch, *et al.* [2] in analytical forms such as Gaussian and Dual-Pearson distribution functions. Some process simulators such as UTMARLOWE and SUPREM perform Monte-Carlo analysis to predict as-implanted dopant profiles and use physical models to simulate the effect of thermal anneals [3,4,5]. In this work, we propose a simple phenomenological approach for predicting dopant profiles at the end of an anneal sequence for a limited range of implant conditions using response surface method (RSM) approach. This method also simplifies the incorporation of different profiles into the device simulators by providing an analytical profile description instead of solving for the profiles numerically as done by many process simulators. The profiles are described using multiple Gaussian distribution functions, which offer an additional advantage of simplifying the analytical modeling of further thermal anneals. The biggest advantage of this method comes from the parametric description of the profiles making it possible to "optimize" the

profiles for required device performance. The process engineers can also use this method in a production facility to quickly and easily predict the effects of implant variations/drifts on the device performance.

## METHODOLOGY

The methodology can be applied for channel and source-drain regions of the transistor also, but in this paper we will limit our discussion to 1-D dopant profiles (along the depth axis) in the MDD and pocket regions of NMOS and PMOS transistors. First, appropriate ranges of various implant conditions were chosen based on the previous experience with similar transistor designs. The ranges chosen were arsenic (2e14-1.2e15 ions/cm2, 10-30keV), boron (4e12-3.2e15 ions/cm2, 10-30keV), BF2 (2e14-1e15 ions/cm2, 10-30keV), phosphorus (2e13-8e13 ions/cm2, 40-100keV). Design of Experiments (DOE) techniques were used for choosing a set of implant conditions required to capture the effect of all settings and any interactions between them. The samples were prepared by implanting the impurities at these dose and energy settings in <100> silicon wafers through appropriate screen oxides. Both NMOS (with boron and arsenic implants) and PMOS wafers (with phosphorus and BF2 implants) were annealed with RTA. These samples were then analyzed using secondary ion mass spectroscopy (SIMS). Figure 1 shows the flow-chart of the methodology used for extracting parameters using these SIMS data and developing process modules. The details of each step in the methodology are discussed in the following sub-sections.

### Profile Description

Figure 2 shows a representative SIMS profile of boron (used as pocket implant for NMOS transistors) in the presence of an arsenic implant. Three gaussian profiles are used to fit the entire SIMS profile for boron concentrations above 1E16 ions/cm2. The profile obtained by adding the three gaussians is also shown. As can be seen from the figure, a good fit is obtained. Thus, boron profile is initially described by 9 parameters; 3 for each gaussian distribution function, viz. dose (D), range (Rp), and straggle (Sp). The total concentration at depth x is then given by:

$$N(x) = \sum_{i=1}^{n} \frac{d_i}{Sp_i \cdot \sqrt{2\pi}} \cdot \exp\left( -\frac{(x - Rp_i)^2}{2 \cdot Sp_i^2} \right)$$

Note that, each gaussian represents a physical aspect of the profile. It has been demonstrated that the crystal damage caused by implanting a heavy atom such as arsenic results in the redistribution of boron atoms. Boron atoms move from certain regions and accumulate near the maximum damage region. Note that gaussian #3 in Fig. 2 has negative values. Moreover, the total dose (calculated by integrating the gaussian function) of gaussian #3 is equal in magnitude to gaussian #1. This clearly takes into account the fact that boron from region #3 has moved to region #1 during RTA. Thus, in Fig. 2, $D_3 = -D_1$, and the total implanted dose = $D_2$. Figure 3 shows the measured (SIMS) and fitted profiles for arsenic concentration in the MDD region of NMOS transistor.

### Parameter Reduction

For a fixed anneal sequence, some of the profile parameters are found to be correlated to the other parameters. Thus, all the Gaussian distribution parameters may not be necessary to uniquely define the profile in the range of implant conditions under consideration. Small number of parameters simplifies the optimization problem substantially. Ideally, the number of independent profile parameters should be equal to the number of process settings that are varied. Hence we model some of the parameters as RSM functions of others. For example, in the case of boron profile for NMOS pocket, we were able to establish following relationships:

$Sp_1 = \text{constant},$

$$Sp_3 = \sum_{i=0}^{n} a_i \cdot (Sp_2)^i,$$

$Rp_2 = \text{constant},$

$Rp_3 = \text{constant},$

$D_3 = -D_1.$

Figure 4 shows the dependent parameters as functions of the independent ones. In this case, independent parameters are $Rp_1$, $Sp_2$, $D_1$, & $D_2$. The above equations were obtained using statistical fitting techniques with $R^2 > 0.98$ and residuals < 0.1%. Thus, we reduced the number of independent parameters required to uniquely define a boron profile to 4. Note that above equations that helped us reduce the number of parameters is valid only over the range of process settings we examined.

Similar parameter reduction method was applied to the remaining three sets of profiles, viz. arsenic, boron (PMOS MDD), and phosphorus. An independent set of parameters was determined for each set. Some of the resulting plots are shown in Fig. 5.

### Process Module

Process module is defined in Fig. 6. It is a set of analytical equations that relate the profile parameters described in the previous section to the process settings, which are implant conditions in this case. For example, the process settings for an NMOS pocket module would consist of boron

dose, boron energy, arsenic dose, and arsenic energy. Note that all other process settings that are kept constant, such as anneal temperatures and times, screen oxide thickness, etc. are not needed as inputs to the process module. Outputs of the process module, viz. profile parameters are modeled as RSM functions of the process settings, i.e.

$$Rp_1 = f(As\_dose, As\_energy, B\_dose, B\_energy),$$
$$Sp_2 = f(As\_dose, As\_energy, B\_dose, B\_energy),$$
$$D_1 = f(As\_dose, As\_energy, B\_dose, B\_energy),$$
and
$$D_2 = f(As\_dose, As\_energy, B\_dose, B\_energy)$$

After statistical analysis, it is found that some of these profile parameters are strong functions of only some of the process settings and not all of them. Hence, the process module equations are reduced to:

$$Rp_1 = f(As\_energy),$$
$$Sp_2 = f(As\_energy, B\_energy),$$
$$D_1 = f(As\_dose, As\_energy, B\_dose, B\_energy),$$
and
$$D_2 = f(As\_dose, As\_energy, B\_dose, B\_energy)$$

A representative plot of $Rp_1$ vs. arsenic implant energy is shown in Fig. 7. The fits for above equations were obtained using statistical fitting techniques with $R^2 > 0.98$, and residuals < 0.1%. In the boron pocket example, note that $Rp_1$, which is the location of the first peak of boron concentration profile, is dependent only on the energy of arsenic implant. This further supports the evidence for boron pileup due to arsenic damage discussed earlier. Also the profile straggle, $Sp_2$, depends only on the energies of the two implants. Similar plot is shown in Fig. 8 for parameter $Sp_2$ of the phosphorus profile in PMOS pocket region.

Clearly, the set of parameters obtained by fitting to SIMS profiles is not unique. The solution depends on the initial guess. We can take advantage of this fact to increase the accuracy of RSMs. Once RSMs for the independent parameters are obtained, we predict the values of these parameters using these RSMs for the set of process settings for which we have SIMS data. We then fix these values of independent parameters and repeat the parameter extraction sequence (fitting) for dependent parameters as explained in the "Profile Description" section. We then repeat the RSM building process for dependent parameters as discussed in the "Parameter Reduction" sequence. This results in a set of RSMs with reduced residuals thereby increasing the accuracy of prediction.

Once all these RSM functions have been obtained, they are incorporated into an optimizer. Using these RSMs, the optimizer determines the set of implant conditions that are needed for a given profile. Note that, to obtain a consistent set of boron and arsenic implant settings in case of NMOS devices, a co-optimization of the pocket and MDD modules is necessary. The details of this "back-solving" of process modules used in process synthesis methodology can be found in [6,7].

## Use in Transistor Design

Application of the process modules described in the previous sections to transistor design is discussed here briefly. The details can be found in [6]. NMOS and PMOS transistors are simulated using MEDICI. The device simulator is first tuned using the methodology described in [8,9]. This tuned simulator can now be used to study the effect of 1-D component of the MDD and pocket profiles on the device performance. By varying the values of the independent profile parameters systematically, one can generate RSM models that relate profile parameters to device performances, such as drive current ($I_d$) and threshold voltage ($V_{th}$). These RSM functions make up the "device module" shown in Fig. 9.

The process module discussed earlier and the device module can be used together to study the effect of process settings on device performance. As an example, Fig. 10 shows the effect of pocket and MDD implant doses on $I_d$ and $V_{th}$ of NMOS devices. All other process settings were kept fixed. Using this information, one can determine the MDD and pocket implant conditions needed to obtain any required $I_d$ and $V_{th}$ values. In process synthesis methodology [6,7], the process and device modules are back-solved to determine the set of all process settings that are required to fabricate a transistor that meets the performance specifications.

## SUMMARY

A method to predict the dopant profiles in MDD and pocket regions of CMOS transistors was presented. Multiple gaussian distributions were used to describe experimentally measured profiles at a limited set of process conditions. Phenomenological RSM approach provided an efficient way of modeling profile parameters as functions of process conditions. This method can be used by device designers to study the effect of implant conditions on device performance. It can also be used by process engineers to obtain a very quick prediction of the effect of implant variations/drifts on device performance. This method has following advantages:

1. Computational efficiency due to analytical equations
2. High accuracy over a small range of process conditions due to phenomenological approach
3. Incorporation of some aspects of physical phenomena by appropriate placement of gaussian distributions
4. Ease in further thermal redistribution of dopants using analytical techniques due to use of gaussian distribution functions
5. Ease in incorporation of the modules in optimizers for device design using process synthesis approach.

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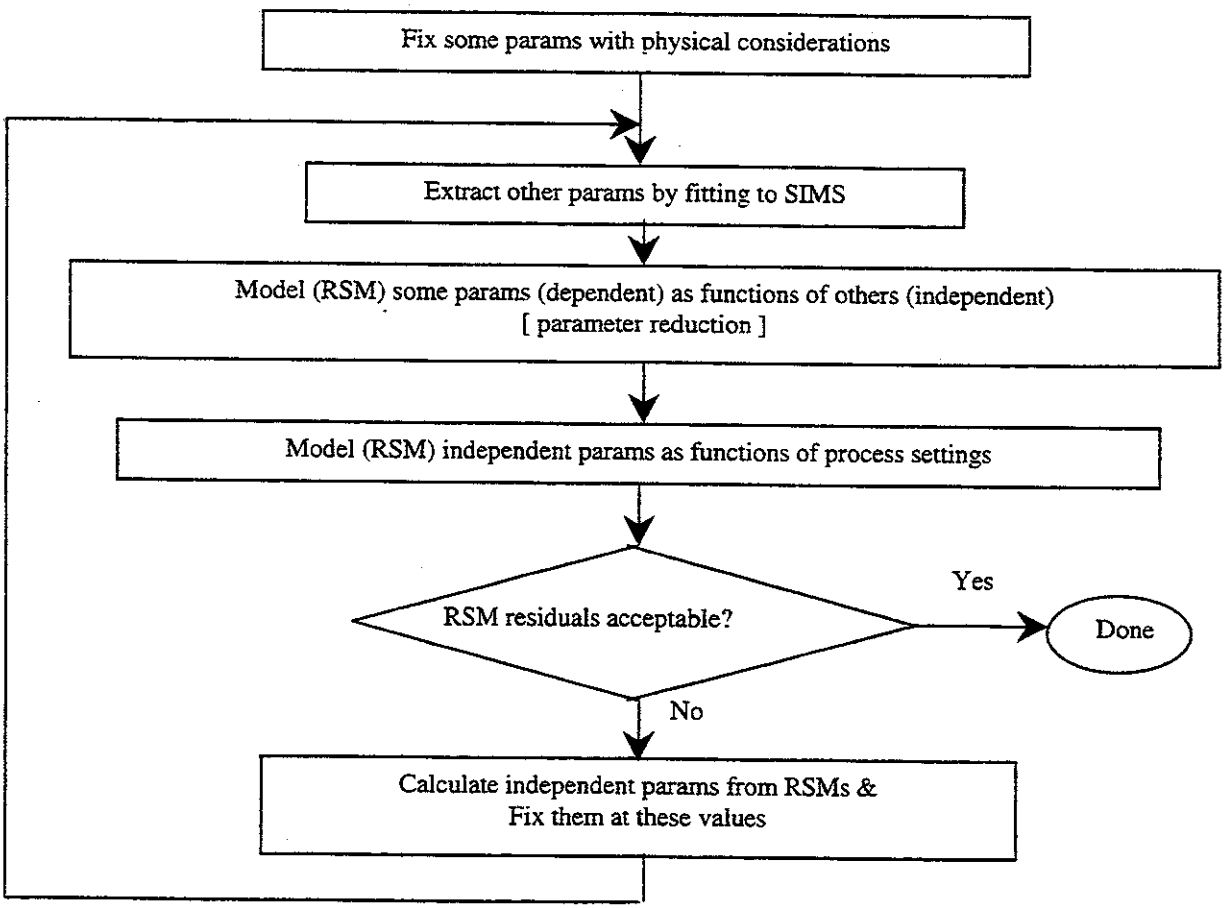


Figure 1. Profile parameter extraction methodology

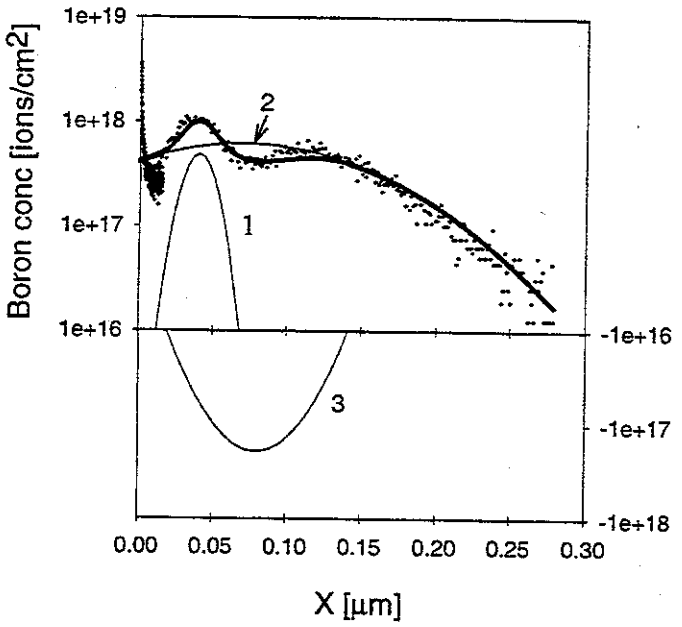


Figure 2. Multi-Gaussian fitting to NMOS Pocket boron SIMS profile. Individual gaussians, viz. two positive and one negative (to represent dopant segregation due to implant damage) are shown with thin lines.

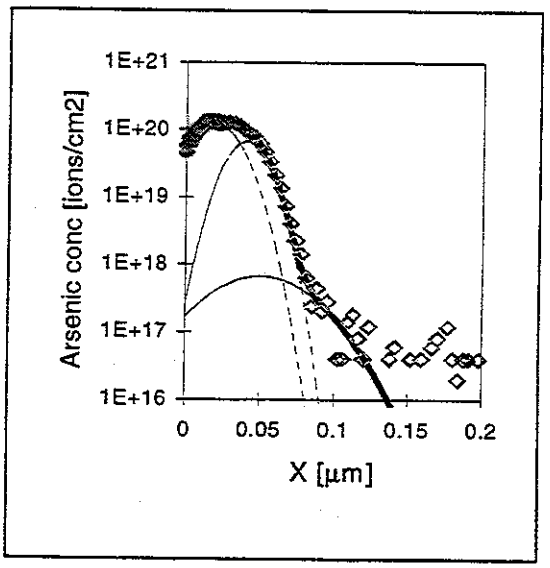


Figure 3. Multi-Guassian fitting to NMOS MDD arsenic profile. Individual 3 gaussians are shown with thin lines.

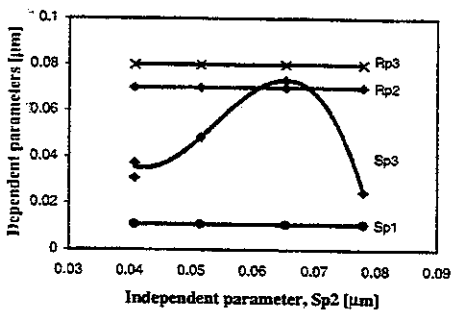


Figure 4. Dependent profile parameters as functions of independent parameter, $Sp_2$, for boron pocket concentration profile

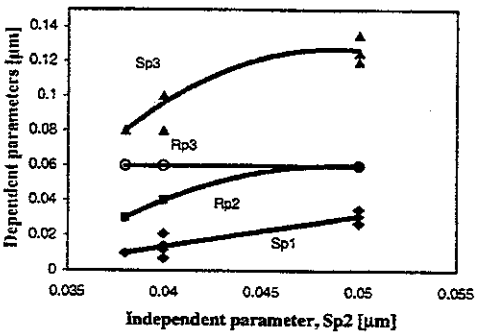


Figure 5. Dependent profile parameters as functions of independent parameter, $Sp_2$, for phosphorus pocket concentration profile

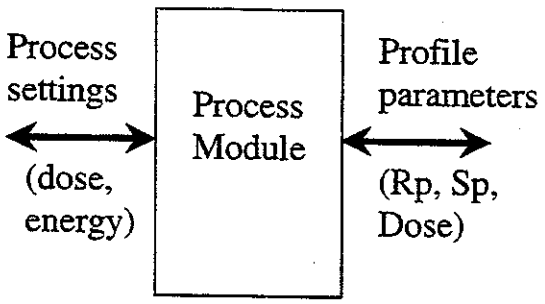


Figure 6. Process Module.

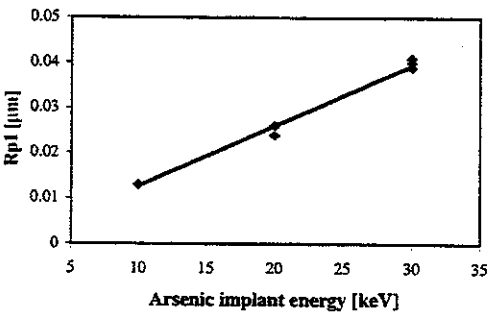


Figure 7. Location of the first Gaussian peak (Rp1) for boron pocket implant as a function of arsenic implant energy

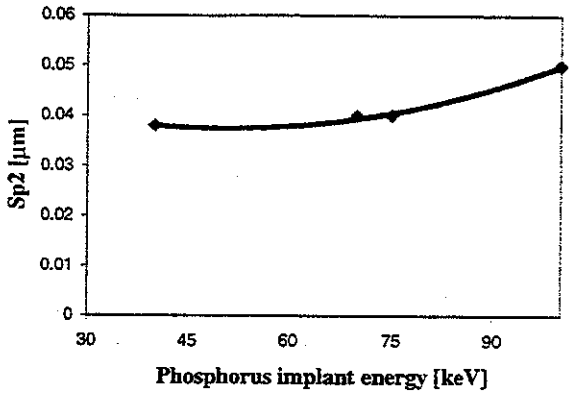


Figure 8. Parameter $Sp_2$ for phosphorus pocket implant as a function of arsenic implant energy

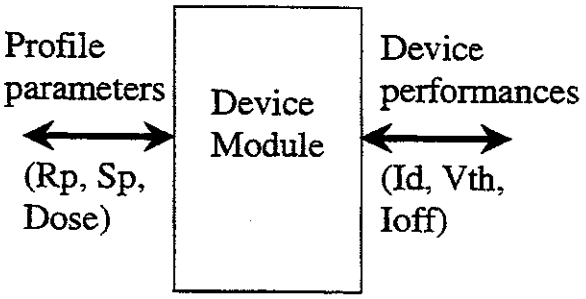


Figure 9. Device Module.

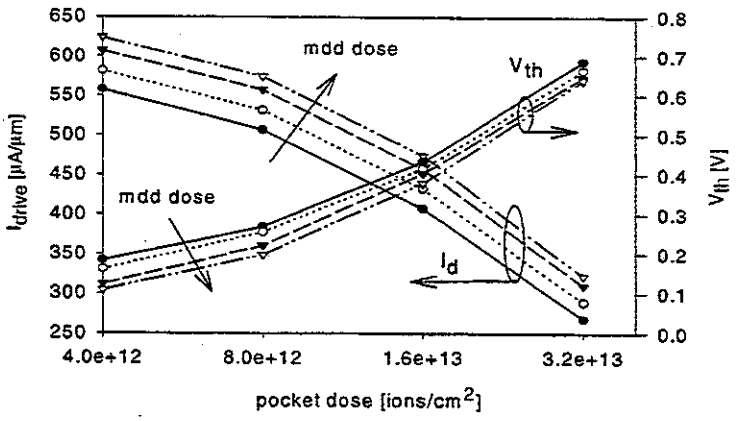


Figure 10. Effect of NMOS MDD and pocket implant doses on device performance.