

## A Monte Carlo Simulation Study of Boron Implants Profiles into NiDoS-LPCVD- Thin Solid Films

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The main aim of our work is to study the influence of different surface treatments that possibly may improve the material properties by using technique of a beam of ions (diffusion – implantation) effecting the distribution of the particles in a semiconductor. As for semi-conductor, we have chosen the polycrystalline Silicon, which is now largely used in micro-electronics field. The importance of this study is related to the ceaseless needs in industry for increasingly reduced, powerful materials and with the smallest possible cost.

Thus, we need to do at first a nitrogen doping process in gaseous phase during the early LPCVD deposition mechanism, which let us obtain the required polycrystalline Silicon films. And then, we have made later an ion implantation process with Boron particles. The results obtained through a Monte Carlo simulation study, although carried out with amounts much lower than what was used in reality, due to computing machine limitations satisfied the predictions assumed in the beginning and encouraged us to continue this study from the point of view of the use of this material, particularly, in VLSI/ULSI various combined systems.

### 1. Introduction

Boron diffusion in silicon thin films is considered as a major problem for fabricating shallow and reliable junctions. Indeed, the MOS transistor used in the realization of circuits devoted to high speed information technology having high performance and promised features should be the key element for the development of microelectronics. This evolution is expressed by the size reduction and the performance enhancement. The dimension diminution involves a gain in speed and a great power in function, but a low cost in fabrication and manufacturing. This miniaturization implies a constant thickness diminution of source and drain junctions to some few nanometres of depth. These junctions are fabricated by ion implantation of dopants followed by an activation thermal annealing treatment.

In this work, we tried to determine the influence of the presence of another dopant in the target on boron diffusion mechanisms into polycrystalline silicon films, and to compare the obtained results to the diffusion profiles, which is obtained by a precise and a reliable experimental technique known as SIMS (mass Spectrometry of secondary ions). This technique has a disadvantage due to its destructive state. The sample analyzed is irremediable lost, and cannot be used later.

The method of simulation that we adopted here is the Monte Carlo method based on the physical models known as the Lindhard, Scharff and Schiff

(LSS) model [1]. This method, which directly reflects the random nature of the diffusion process, gave good results that are very illustrative and comparable to the experimental results [2]. The program that we used is based on the TRIM (Transport of Ions in Matter) concept [3]. It gives information on the distribution of boron implants and the prediction on the manner how these dopants diffuse inside the target material.

### 2. Results and discussion

Some simulated results, obtained by means of our data processing tool, are given in this section. Starting from a calculation programme based on the TRIM code, we considered three cases of samples, the first sample is a target of silicon boron doped, which will be used as reference compared to the two other samples. The second sample is made during the phase LPCVD deposition process giving a polycrystalline silicon film, in situ nitrogen doped. And the third sample is boron implanted.

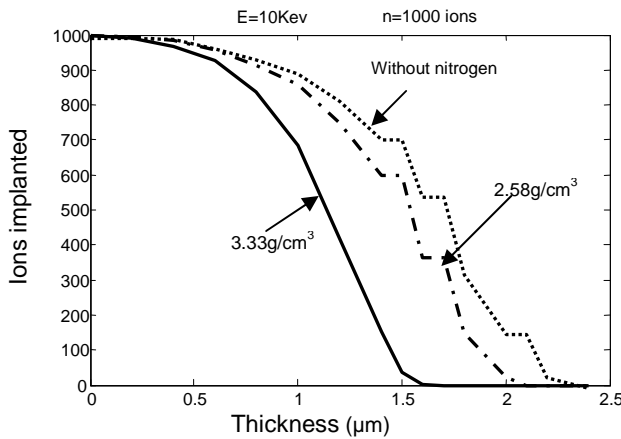
In order to make a comparison and to study the influence of the nitride effect on the penetration depth of incident particles, we should proceed as follow:

We define  $A_1$  and  $Z_1$ , as the mass and atomic number of the target atom (Silicon),  $A_2$  and  $Z_2$  as mass and the atomic number of the atom constituting the incident beam and  $A_3$  and  $Z_3$ , as the mass and the atomic number of the atom doping the target (Nitrogen).

The presence of nitrogen in our simulation program is defined by the variation of the target density, the value of this density for selected cases correspond to real value of the total nitrogen concentration which was experimentally introduced into the sample. The values indicated on the curves correspond, in fact, to the following concentrations:

$$\begin{aligned} \rho=2.58 \text{ g/cm}^3 &\longrightarrow c=7.9 \cdot 10^{20} \text{ at/cm}^3 \\ \rho=3.33 \text{ g/cm}^3 &\longrightarrow c=3.1 \cdot 10^{21} \text{ at/cm}^3 \end{aligned}$$

In Fig. 1, we present some results obtained which show that the Monte Carlo method is well adapted model to simulate the ionic trajectories of implants. This way yields to reconstitute the dopant profile leads a direct access to some decisive parameters on the control of ion implantation



process applied for microelectronic materials. Fig.1: Comparison between the simulated profile results for input data (n= 1000 Boron ions, E=10 KeV), in the cases of a sample un-doped Nitrogen and two samples in situ Nitrogen doped for two values of density: 2.58 g/cm<sup>3</sup> and 3.33 g / cm<sup>3</sup>.

From these curves, we suppose that the diffusion of nitrogen in the polycrystalline structure inside the grain boundaries satisfies the changing structure due to the defect mechanism activation, in particular, the grain boundary is the place where complex phenomena such as segregation, precipitation, discontinuity in the directions of magnetization etc. Occur. It is one of the principal defects which cause major problems in the polycrystalline semiconductor behaviour [4].

To consolidate our study, we have also tried to study the effects of some parameters such as the energy and the amount of ion implantation on the profile behaviour.

In table-1, we gave results for three values of energy, and we recorded the maximum thickness of penetration of 100 Boron ions in the three cases of

the studied samples. We see clearly that for the sample not nitrogenated, the ions travel in depths is much more significant than for the other nitrogenated samples. This is for the three values of the implantation energy.

We have also tried to study the influence of another control parameter of the ion implantation, which is the amount of ions needed for the calculations. For our data processing tool, tests are made choosing an average of five hours for 1000 particles and sometimes more. A big amount of particles should be very attractive to complete this present work. The results obtained are illustrated in Table 2. Nevertheless, we note that for the value of 1000 particles, the thicknesses reached are lower than those of 100 particles.

It is always the thicknesses of the nitrogenated samples which is lower as compared to those of the sample not nitrogenated at all.

Table 1: Influence of the ionic energy of implantation on the profile diffusion of boron implants.

Incident energy	10 KeV	25 KeV	50 KeV
Without nitrogen	3.6411 µm	15.6827 µm	68.1565 µm
With nitrogen c=7.9*10 <sup>20</sup> at/ cm <sup>3</sup>	2.0523 µm	10.5851 µm	37.3484 µm
With nitrogen c=3.1*10 <sup>21</sup> at/ cm <sup>3</sup>	1.5901 µm	7.9332 µm	28.9366 µm

Table-2: Influence of the dose implants on the profile simulation results.

Boron Ions	100 ions	1000 ions
Without nitrogen	e=3.507µm	e=2.195µm
With the nitrogen c=7.9*10 <sup>20</sup> at/ cm <sup>3</sup>	e=1.793µm	e=1.597µm
With the nitrogen c=3.1*10 <sup>21</sup> at/ cm <sup>3</sup>	e=1.575µm	e=1.198µm

### 3. Conclusion

The main aim in our work was to study the influence of a co-doping effect on the diffusion mechanisms of ionic particles inside a polycrystalline layer. Indeed, the ionic trajectories reconstituting the profiles obtained show a good agreement with profiles experimentally obtained. Theoretical and experimental results agree in all the cases studied including a dense target, a layer previously doped with another element and a layer previously doped with two different elements. The collision interactions involve braking effects and give the random deviation of the trajectories. The

other promising point is that an appreciable reduction in the thickness of penetration in the samples containing the element that are nitrogenated in comparison to those samples that are not nitrogenated.

Thus, these results obtained encourage us to continue further studies and to complete future calculations of phenomena of diffusion and binary collisions.

#### 4. References

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