Effects of Boron diffusion on Titanium silicide formation

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***Abstract*—Secondary ion mass spectrometry (SIMS) has been used to investigate Boron diffusion in Titanium silicide layers for several annealing conditions of duration and temperature. Experimental profiles were simulated using a model based on the famous Fick's laws and the effect accompanying boron diffusion during silicidation like segregation and clustering. The comparison between simulation results and those of the literature in the same annealing conditions shows a good agreement between our results and those of other works. This explains that boron diffusion in titanium silicide depends on segregation, clustering and the solid solubility exceeds.**

Keywords—SIMS, Titanium Silicide, Boron, simulation, diffusion.

I. INTRODUCTION

Currently, using Titanium silicide as contact and interconnection in the industry of CMOS technology faces a difficult trade-off between thickness and sheet resistance. The contact junction depth must still scale with gate length. To avoid high contact resistance and high contact leakage, no more than half the contact junction depth can be consumed in the formation of the silicide. Therefore, the silicide must become progressively thinner to accommodate the more shallow contact junction for scaled contacts [1].

In this work, we present an attractive candidate the Titanium silicide with each interesting characteristics: low resistivity, low silicide formation temperature and good thermal stability [2]-[3].For our samples Titanium silicide boron doped we used a serial of heat treatment with RTA and STA.The rapid heating is an attractive method to reduce thermal budget and shallow junction [4]. Indeed J. Du et al [3] show that the conductivity of the thin films increases with the increase in the content of $TiSi_2$ crystalline phase.

Secondary Ion Mass Spectrometry (SIMS) technique was used to investigate boron diffusion in the Titanium silicide layer before and after annealing. However, it is necessary to simulate the resulting profile in order to understand the effects of boron on silicidation and to predict accurately the dopants shapes in any annealing conditions. It is know that the effect of silicidation is the induction of segregation of dopants. This is an important factor for governing transport and contact resistance of MOSFET devices [5]. This paper presents a comparison between experimentation and simulation of boron diffusion in Titanium silicide formation. The SIMS profiles were obtained by analysis different structures of boron in Ti/Si structure in different operative conditions using a Cameca-*Ims3f* instrument at oblique incidence. The simulation is founded on numerical model based on the Fick's law and the effects of dopants segregation and accumulation before and after annealing. This leads to simulate boron diffusion in Titanium silicide and to obtain several parameters which control the phase's evolution of this kind of silicide..

II. EXPERIMENTAL PROCEDURE

In order to obtain concrete results we used a serial of heating treatments short and rapid annealing and several temperature values to understand much more the effect of boron diffusion on silicidation.

TABLE I. DESCRIPTION OF THE ANNEALING CONDITIONS

Samples	Conditions	
	Temperature (°C)	***Duration (min)***
1	710	3
2	710	7
3	710	9
4	680	11
5	680	20
6	680	25

III. NUMERICAL METHOD AND MODELING

Diffusion is a physical phenomenon controlled by the famous Fick's laws and characterized by the tendency of doping species to spreading out. Ionic implantation is the most famous process used to introduce the doping species in the microelectronic industry. In very high doping level, the limits of solid solubility in silicon can be reached and have atoms trapped in interstitial and lacunars sites. This phenomenon will be modeled using the SIMS profile and simulation of the diffusion evolution according to different annealing parameters, i.e., temperatures and durations.

A. The Proposed Model

In the few last years there was a renew interest to control the dopants segregation in the silicide as the devices sizes reducing [5]-[6]-[7]. To understand the diffusion mechanism accompanying silicidation phenomenon, in this work, we present a new study based on real SIMS profiles obtained in different conditions, i.e., various temperature and heat duration.

Starting with the calculation of the solid solubility limit, whichexpressed by the following estimated equation given by Solmi et al [8]:

$$C_{Sol}=9{,}25.10^{22}\exp\left(\frac{0{,}73}{K_B.T}\right), \quad (1)$$

With KB: Boltzmann's constant (J/°K) and T: annealingtemperature in Kelvin.

With the high doping concentration, solid solubility level can easily exceeded and the damage created by the ionic implantation leads to many phenomena like segregation, cluster formation and dopants trapping.

The proposed model based on the famous Fick's law with a combination of different equation traducing dopants segregation, clustering formation and trapping.

$$\vec{F_b} = -D_b \frac{\partial C_b(x,t)}{\partial x}, \quad (2)$$

In transitory mode, we have:

$$\frac{\partial C_b(x,t)}{\partial t} = -\frac{\partial F_b}{\partial x}, \quad (3)$$

C b: concentration of an impurity " B ".
Fb: flow of an impurity "B".
Db: the diffusion Coefficient.

The combination on the equation (2) and (3) we have the third Fick's law:

$$\frac{\partial C_b(x,t)}{\partial t} = -D_b \frac{\partial^2 C_b(x,t)}{\partial x^2}, \quad (4)$$

Generally, the vacancy diffusion is dominating, and the diffusion coefficient becomes proportional to the vacancy density [9].

The concentration of the ionized impurity C_b^* and the total impurity concentration Cb, were linked by $C_b^* = \alpha C_b$ α: activation level of the doping agent (0 ≤α≤ 1).
α = 1: toutes les impuretés sont ionisées.
α = 0: les impuretés sont totalement inactives.
Therefore, we will have:

$$S_B = \frac{1}{1+2m^2\left(\frac{\alpha_B C_B}{C_{sol}}\right)^{2m-1}}, \quad (5)$$

It is noticed that the trapping factor is directly related to the concentration C, by α, the size of the clusters m, and concentration of significant balance of a beginning of clusters formation C_{sol}. This factor reduces the diffusion coefficient considerably in high doping level.

Gaps influences (β): There are several types of diffusion (vacancy, interstitial ...), usually vacancy diffusionis the dominant phenomenon, and the diffusion coefficient becomes proportional to the vacancy density [9].

$$D=D_i^0V^0+D_i^-V^-+D_i^+V^++D_i^{-2}V^{-2}+..., \quad (6)$$

With: D_i^0, D_i^-, D_i^+, D_i^{-2} : intrinsic diffusivity.
V^0, V^-, V^+, V^{-2} : Standard gaps concentrations.

The effect of gaps occurs by the presence of a deficient state of multiply charged impurities, where the diffusion is assumed to be performed by the interaction of set of diffusers [10].

At the thermodynamic equilibrium, a number of deficiencies still exist, because the energy is increased by the presence of a disorder in the structure. The probability that we have a vacant site is given by the Boltzmann equation [11]:

$$p=\exp\left(-\frac{E_V}{K_BT}\right), \quad (7)$$

EV: is the required energy to bring an atom of a busy site that is a neighboring site; it depends on the position of the Fermi level Ef.

$$\frac{C_l}{C-C_l}=\exp\left(-\frac{E_V}{K_BT}\right), \quad (8)$$

C is the total concentration of atoms; C_L is the concentration of vacancy. The vacancy density for a given state of charge depends on the temperature; it is given by [12]:

$$C_L=C_i\exp\left(\frac{E_f-E_i}{K_BT}\right), \quad (9)$$

Ci: is the intrinsic vacancy concentration, E_f: the intrinsic Fermi level.

From the third Fick's law, we have:

$$\frac{\partial C_b}{\partial t}=-\frac{\partial}{\partial x}\left[-D_i\frac{1+\beta f_b}{1+\beta}\left(\left(1+\frac{\alpha C_b}{\sqrt{(\alpha C_b)^2+4n_i^2}}\right)\frac{\partial C_b}{\partial x}\right)S_B\right], \quad (10)$$

$$f_b=\frac{p}{n_i}=\frac{2n_i}{\sqrt{(\alpha C_b)^2+4n_i^2}-(\alpha C_b)}$$

B. Initial conditions

Equation (10) represents the general expression of the proposed model. To solve problem with a partial differential equation, we have used a numerical method which is the finite differences. The initial and the limit conditions are determined from Fig. 1which shows a good adjustment between SIMS profile and the simulated one used as initial conditions. According to the study done by Solmi et al [8], we have used a combination of two half Gaussian function with various experimental parameters,

$$N=C_P\exp\left[-\frac{(X-R_P)^2}{2\Delta R_P^2}\right], \quad (11)$$

N is the concentration (at/cm3)
Cp isthe ion implantation dose, Rp is the projected Range, and ΔRp the standard deviation [13].

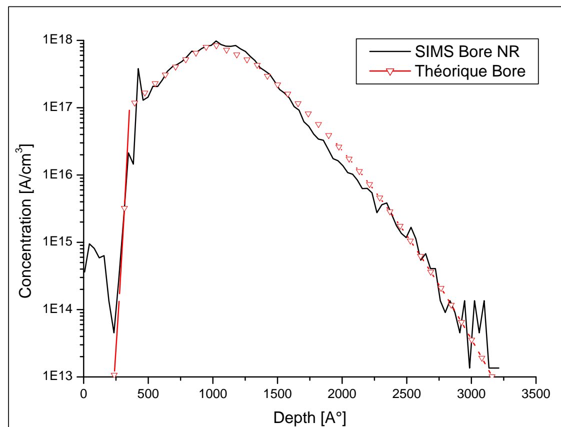


Fig. 1. Theoretical and experimental SIMS Boron profile Before annealing

IV. RESULTS AND DISCUSSION

A. Simulation Of SIMS Profiles

Figure 2 presents real SIMS profiles of boron in TiSi2structureand the simulation in different annealing conditions (various values of temperature and duration). It show a great agreement between simulation and SIMS profiles.

We can notice two different gaits: the double slope and a Gaussian shape :

The shape of Boron profile after annealing depends on several factors:

Peaks boron in the silicide film and a much larger out diffusion length. This may be caused by the higher boron diffusivity in both materials.

Silicidation inducessegregation ofdopant, so the boron distribution is not uniform.

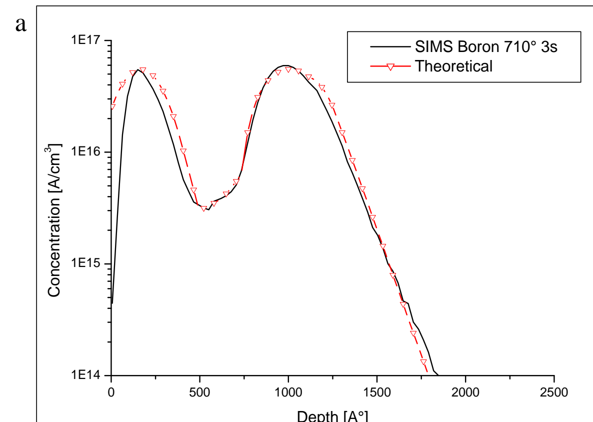
The defects in the metal.

From R.Beyrs [14] in the high doping case we have the formation of some precipitates like the TiB wich induces a fence to silicon diffusion so it can stop the moving from C49 to C54 phases.

According to these details, the diffusion of boron in titanium silicide depends on several phenomena:

- Dopants segregation clustering and the vacancies.
- The solid solubility exceedance.

a



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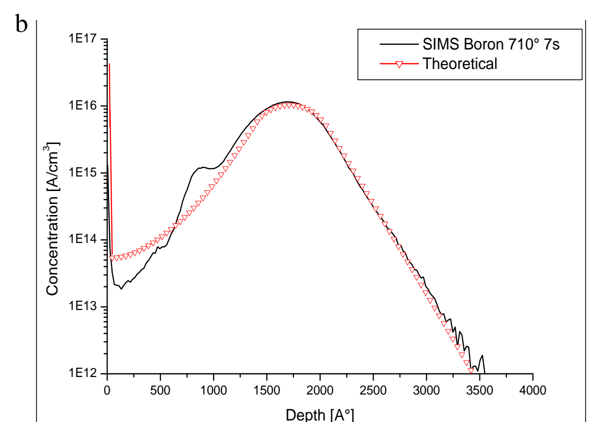

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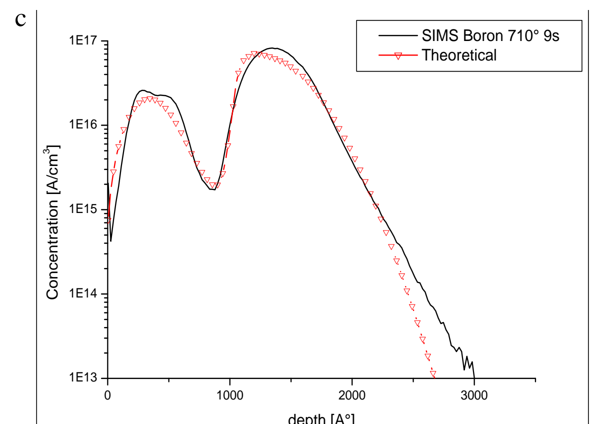

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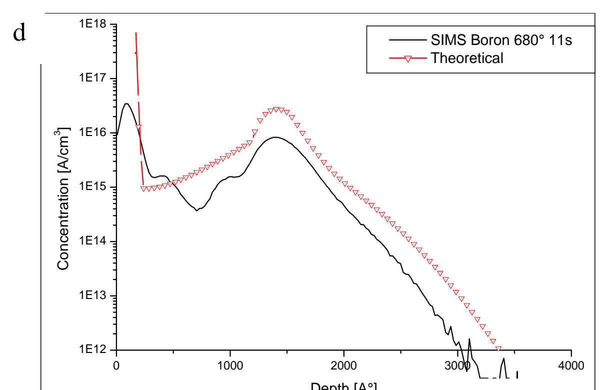

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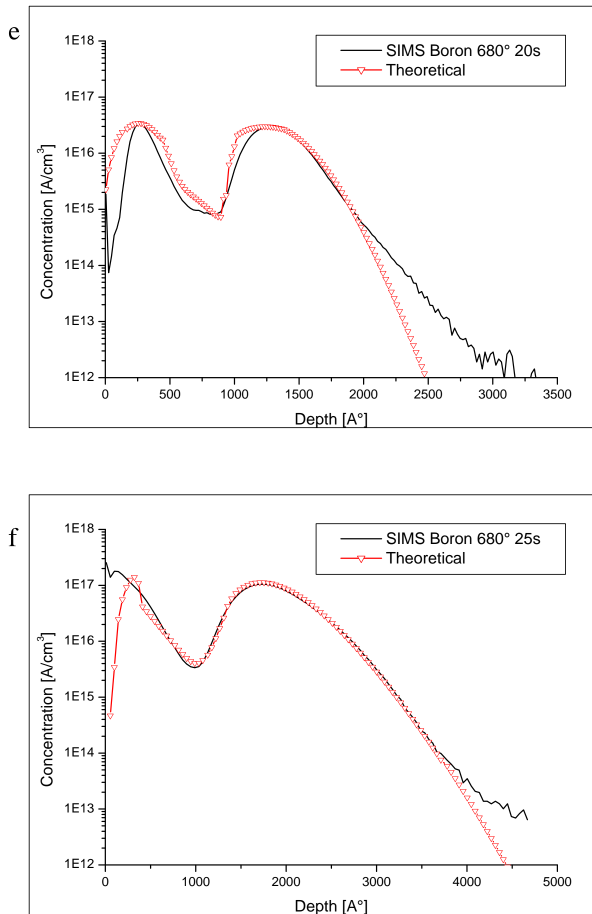

Fig.. 2. Simulation of SIMS profiles: (a), annealing 710°C, 3s (b), annealing 710°C, 7s (c),annealing 710°C, 9s (d), annealing 710°C, 11s (e), annealing 710° C, 20s (f), annealing 710°C, 25s.

According to the work of R. Pretorius [16] the diffusion coefficient of the boron in TiSi2 is around 10-13 cm2/s at 600°C so it's close to our result obtained at 680°C

- β Was chosen to equal 0.11, Girault et al [14] advice to take β : 0.1 to 0.3.

- The fraction of activated dopants α is about 20% in the majority of samples and Zhao et al [17] shows that αmust be higher than 18%.

TABLE II. SIMULATION RESULTS

Samples	**Conditions**		
	Temperature (°C)	***Duration (min)***	***Diffusion coefficient Cm²/s***
1	710	3	$1,3344.10^{-12}$
2	710	7	$3,7308.10^{-11}$
3	710	9	$1,7522.10^{-12}$
4	680	11	$3,8197.10^{-12}$
5	680	20	$7,7311.10^{-12}$
6	680	25	$6,0164.10^{-12}$

CONCLUSION

Secondary ions mass spectrometry technique have been used to investigate Boron diffusion during silicidation for several annealing duration and temperature. The simulation is based on numerical method which is finite differences. It is shown a great agreement between simulation and experimentation. This accordance led to determine several parameters, which explain the comportment of boron in $TiSi_2$ structure during different phases of silicidation. In particular, the shape of boron distribution profilein titanium silicide depends on several structural factors as well as annealing conditions, i.e. segregation, presence of defects, the solid solubility, exceedance, etc.

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