

## SIMULATION OF CARBON ION PLANTATION IN SILICON TARGETS

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### Résumé

Dans ce travail, plusieurs phénomènes liés à l'implantation ionique du carbone, dans des cibles amorphes de silicium, ont été simulés. L'étude est réalisée par le code TRIM ou SRIM pour une dose de  $2.7 \times 10^{17} \text{ C}^+ \text{ cm}^{-2}$  et une énergie de 80 keV. Plusieurs quantités (le parcours projeté ( $R_p$ ), la déviation standard ( $\Delta R_p$ ), etc.), caractérisant l'implantation ionique, ont été obtenues et comparées avec la littérature. D'autre part, les défauts d'irradiation (lacunes et phonons) dans les cibles ont été prédits. Concernant la redistribution des ions  $\text{C}^+$ , une bonne corrélation entre la simulation et la littérature a été révélée. Cependant, on doit noter que l'influence de certains facteurs (la température du recuit, l'orientation cristallographique du substrat, etc.) sur les phénomènes étudiés ne peut pas être prévue par le code utilisé.

**Mots clés:** carbone ; silicium ; implantation ionique ; simulation.

### Abstract

In this work, several phenomena related to carbon ion implantation, in amorphous silicon targets, were simulated. The investigation was performed using the TRIM code for a dose of  $2.7 \times 10^{17} \text{ C}^+ \text{ cm}^{-2}$  and an energy of 80 keV. Several quantities (the projected range ( $R_p$ ), the standard deviation ( $\Delta R_p$ ), etc.), characterizing the ion implantation, were obtained and compared with literature. On the other hand, the radiation damage (vacancies and phonons) in the substrates was also predicted. Concerning the redistribution of  $\text{C}^+$  ions, a good correlation between the simulation and literature has been revealed. However, we note that the investigation of the effect of some factors (annealing temperature, crystallographic orientation of the targets, etc.) on the studied phenomena is not possible by the TRIM code.

**Keywords:** carbon; silicon; ion implantation; simulation.

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### ملخص

في هذا العمل قمنا بمحاكاة عدة تفاعلات خاصة بالزرع الأيوني للكربون داخل مساند من السليسيوم غير المتبلور. تمت الدراسة على التوالي. تحصلنا على عدة قيم 80 keV و  $2.7 \times 10^{17} \text{ C}^+ \text{ cm}^{-2}$  من أجل جرعة و طاقة تساويان TRIM بواسطة البرنامج و قارناها مع المراجع المتوفرة. من جهة أخرى تنبأنا بالعيوب خاصة بالزرع اليوني) الخ  $\Delta R_p$ , الانحراف,  $R_p$  المسار ( تحصلنا على توافق جيد بين المحاكات و  $\text{C}^+$ (الفجوات و الفونونات) الناتجة عن الزرع الأيوني للكربون. بالنسبة لتوزيع أيونات الخ) غير ممكن باستعمال, التوجه البلوري للمساند, المراجع. لكن يجب القول بأن تأثير بعض العناصر (درجة حرارة المعالجة TRIM البرنامج.

كلمات مفتاحية : كربون ; سليسيوم ; زرع أيوني ; محاكاة.

I – INTRODUCTION

Ion implantation is a technique widely employed to introduce dopants, in semiconductor substrates, for the fabrication of integrated microcircuits [1]. This is due to the fact that this process is able to provide excellent spatial and dose control. Actually, this method is used in different domains because it leads to the modification of the materials surfaces [2]. The range profiles and the stopping of energetic ions in the targets have been largely investigated by researchers. They have used several theoretical approaches and many sophisticated experimental techniques. Indeed, when energetic ions penetrate in the solid, many target atoms are knocked off their initial positions which generate many interstitials and vacancies in the substrate lattice. Moreover, actually, the ion implantation is employed to produce shallow layers which present a good continuous transition in depth. As an application of this effect in microelectronics industry, the researchers use the impl layers as buried conductors or shallow pn-junctions. instance, many studies are oriented to synthesize embe silicon carbide in silicon specimens using high doses of ca ions [3,4]. The silicon carbide has attracted many into because of its attractive properties at extreme conditio: temperature, power and radiation [5,6]. In this work, we the carbon ion implantation in silicon targets. The investig is performed by simulation using the upgraded T (TRansport of Ions in Matter) [7] version, SRIM (Stopping & Range of Ions in Matter) [8]. Our investigation is emphasized on the prediction of carbon concentration-depth profiles, energy loss of ions and radiation damage

2- Implantation technique

When energetic ions are introduced into a target, electronic and/or nuclear collisions are generated between the incident ions and the target atoms. According to the ions energy, several phenomena may occur [9]: backscattering of ions, emission of light and/or secondary electrons, formation of aggregates, emission of secondary ions and the implantation of ions (Fig. 1, left).

Concerning the redistribution (n(x)) of the ions in the target, the simplest approximation is the Gaussian distribution [10]

which is described by the two moments ( $R_p$  and  $\Delta R_p$ ) and given by the function:

$$n(x) = n_0 \exp \left( \frac{-(x - R_p)^2}{2 (\Delta R_p)^2} \right)$$

$$n_0 = \frac{\Phi}{\sqrt{2\pi} \Delta R_p}$$

where  $\Phi$  is the ion dose per unit area,  $R_p$  and  $\Delta R_p$  are the projected range (average depth from the surface) and the standard deviation (half width at half maximum) respectively (Fig. 1, right).

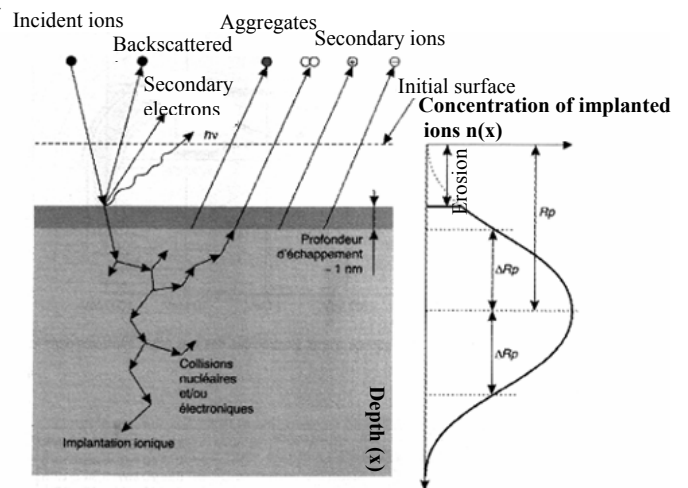


Figure 1: Scheme of the different phenomena occurring during the interaction of incident ions with a target (left).

Gaussian redistribution of implanted ions (right) [9, 10]. However, if the redistribution (or profile) of ions deviates from the ideal Gaussian, the approximation of Pearson is used [9]. For such approximation, two parameters (or moments) are added. They are the skewness ( $\gamma$ ) and the kurtosis ( $\beta$ ). We note that  $\gamma$  is a measure of the profile tendency to lean toward or away from the surface. Concerning the  $\beta$  moment, it is the measure of the profile flatness [9].

**3- Simulation technique**

The SRIM2006 [8] was used to simulate the interactions of carbon ions with silicon targets. It is a group of programs able to compute the stopping and range of ions (10 eV - 2 GeV/amu) into matter using a full quantum mechanical treatment of ion-atom collisions. The calculation is based on statistical algorithms in which it is assumed that the ion and atom have a screened Coulomb collision including interactions between the overlapping electrons shells [11]. In the calculation, it is assumed that the atomic density of the target remains constant during the implantation process. We used incident carbon ions, a silicon target (10000 Å) and “Detailed Calculation with full Damage Cascade” option. In this option, every recoiled atom is followed until its energy drops below the lowest displacement energy of any silicon atom. The values of the displacement energy ( $E_d$ ) (of a silicon atom) and the Si binding energy ( $E_b$ ) are 15 eV and 2 eV respectively. These default values given by SRIM are slightly different with regards to tabulated data [12, 13]. Concerning the number of ions, we used 99999 which is the default value proposed by SRIM. However, in some cases, we used 10000 ions for comparison. For the angle ( $\varphi$ ) of implantation, in some cases  $\varphi$  was equal to zero (*i.e.* carbon beam perpendicular to the silicon target). In others,  $\varphi$  was equal to  $7^\circ$  (which is the geometry generally employed during ion implantation operation). Finally, we note that the computation was performed in a personal computer (PENTIUM P4, having a speed of 3.4 GHZ and a RAM of 2 GO).

**4- Results and discussion**

Figure 2 shows the SRIM predictions of nuclear and electronic stopping powers versus the energy of carbon ions. From this plot, one can see that the transfer energy to the silicon lattice is governed by the electronic collisions.

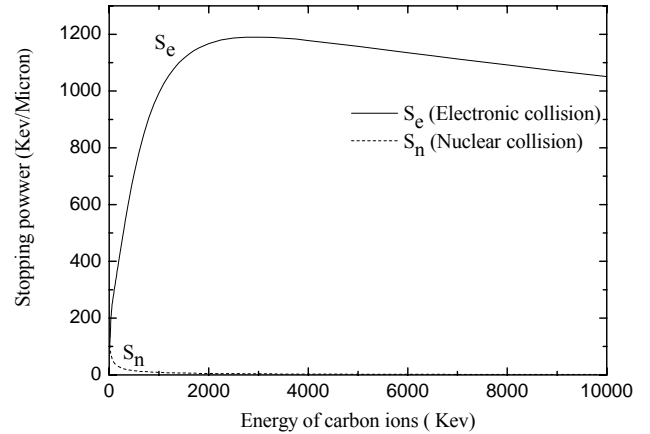


Figure 2: Simulation of the nuclear ( $S_n$ ) and electronic ( $S_e$ ) stopping powers, in a silicon target, for different energies of carbon ion implantation.

In ion implantation, it is crucial to predict the ion implantation parameters such as the range profiles, the projected range  $R_p$  and the standard deviation  $\Delta R_p$ . In figure 3, the distribution of carbon ions in the silicon target (for an energy of 80 keV, a dose of  $2.7 \times 10^{17} C^+cm^{-2}$  and an angle  $\varphi$  of  $7^\circ$ ) is reported. According to this plot, one can notice that the simulated profile has almost a Gaussian form which is in agreement with the experimental study provided in literature [14].

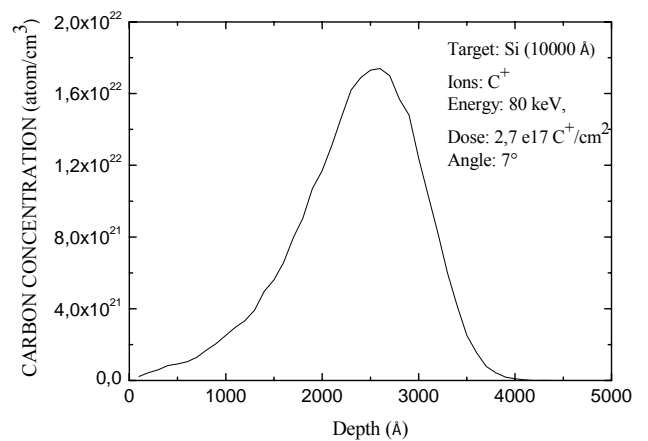


Figure 3: SRIM prediction of carbon ions profile in silicon target.

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The energy and dose are equal to 80 keV and  $2.7 \times 10^{17} \text{ C}^+$   $\text{cm}^{-2}$  respectively.

We note that the distribution was obtained for 99999 ions which were supposed to be oriented with an angle  $\varphi$  of  $7^\circ$  with respect to the silicon surface. The parameters extracted from the profile of figure 3 are as follows: the projected range  $R_p = 2295 \text{ \AA}$ , the standard deviation  $\Delta R_p = 655 \text{ \AA}$ , the skewness  $\gamma = -0.588$  and the kurtosis  $\beta = 3.247$ . First of all, we note that the projected range and the standard deviation are slightly inferior to the experimental value provided in literature [14] (*i.e.*  $R_p = 2600 \text{ \AA}$ ,  $\Delta R_p = 760 \text{ \AA}$ ). We attribute the difference to the fact that the simulated profile has not a perfect Gaussian shape. Indeed the negative value of the skewness indicates that the peak is skewed towards the surface [15]. Whereas, the obtained value of the Kurtosis indicates that a small broad tail is present. Besides, we note that the simulation performed for an angle  $\varphi$  of  $0^\circ$  provided comparable results with those corresponding to an angle of  $7^\circ$  (Tab. 1). This is logical since the SRIM code assumes that the targets are amorphous which means that no channelling effects may be detected.

Method	$R_p(\text{\AA})$	$\Delta R_p(\text{\AA})$	$\gamma$	$\beta$
SRIM ( $\varphi = 0^\circ$ )	2309	655	-0.602	3.2711
SRIM ( $\varphi = 7^\circ$ )	2295	655	-0.588	3.2472
Literature [14]	2600	760	.....	.....

Table 1: Characteristic details of the carbon distribution, in silicon targets, determined by SRIM code for 99999 ions in different conditions ( $\varphi = 0^\circ$  &  $\varphi = 7^\circ$ ).

$R_p$ : the projected range,

$\Delta R_p$ : the projected range straggling,

$\gamma$ : the skewness,  $\beta$ : the kurtosis.

Besides, we note that in SRIM code, two parameters related to the substrate are introduced. The first one concerns the displacement energy ( $E_d$ ) and it defines the quantity (in terms of energy) that a recoil must possess to overcome the lattice forces and to move away from its original position [7,8]. The second parameter concerns the lattice binding energy ( $E_b$ ) and it traduces the energy lost (into phonons) by every recoiling target atoms when it leaves its lattice and

recoils in the target [7,8]. The default values of  $E_d$  and  $E_b$ , for semiconductors, which are included in SRIM, are 15 eV and 2 eV respectively. They are slightly different from those given in literature (*i.e.*  $E_d = 13 \text{ eV}$  &  $E_b = 3 \text{ eV}$ ) [14, 15]. In table 2, we report the values of  $R_p$ ,  $\Delta R_p$ ,  $\gamma$  and  $\beta$  obtained by simulation for the default values of  $E_d$  and  $E_b$  and for the values provided in literature [14, 15]. According to the results reported in table 2, we notice that the simulation performed for the default values of  $E_d$  and  $E_b$ , provides identical results with the simulation executed with the values given in literature.

Method	$R_p(\text{\AA})$	$\Delta R_p(\text{\AA})$	$\gamma$	$\beta$
SRIM ( $E_d=15\text{eV}$ , $E_b=2\text{eV}$ )	2292	654	-0.6131	3.2448
SRIM ( $E_d=13\text{eV}$ , $E_b=3\text{eV}$ )	2292	654	-0.6131	3.2448
Literature [14]	2600	760	.....	.....

Table 2: Characteristic details of the carbon distribution, in silicon targets, determined by SRIM code

( $N = 10000$  ions,  $\varphi = 7^\circ$ ) in different conditions

( $E_d = 15\text{eV}$ ,  $E_b = 2\text{e}$  &  $E_d = 13\text{eV}$ ,  $E_b = 3\text{eV}$ ).

Besides, we note that the default number of ions proposed by SRIM is 99999. In our study, we noticed that this required a long simulation time ( $t=600$  minutes) especially if we chose the ‘‘Detailed Calculation with full Damage Cascade’’ option. For this reason, we tried to use a less ions number (*i.e.*  $N=10000$  ions) to make a comparison. First of all, the simulation time was notably decreased ( $t = 60$  minutes). Concerning the values of  $R_p$ ,  $\Delta R_p$ ,  $\gamma$  and  $\beta$  parameters, they are reported, in table3, for both cases. From this table, we can notice that the results are similar which means that it is possible to reduce the number of ions during the simulation by SRIM.

Method	$R_p(\text{\AA})$	$\Delta R_p(\text{\AA})$	$\gamma$	$\beta$
SRIM ( $N=10000$ ions)	2292	654	-0.6131	3.2448
SRIM ( $N=99999$ ions)	2295	655	-0.5880	3.2472
Literature [14 ]	2600	760	.....	.....

Table 3: Characteristic details of the carbon distribution, in silicon targets, determined by

SRIM code ( $\varphi = 7^\circ$ ) in different conditions  
( $N=99999$  ions &  $N=10000$  ions).

During the ion implantation in solid targets, many defects are enhanced in the material. In this work, we have used the SRIM program to predict the distribution of phonons (Fig. 4) and vacancies (Fig. 5) generated in the silicon target by the implantation of carbon ions (dose= $2.7 \times 10^{17} \text{ C}^+ \text{ cm}^{-2}$ , energy 80 keV). First of all, from these figures, we note that the radiation damage is due to both ions and recoils. But it is clear that the defects (*i.e.* phonons or vacancies) enhanced by recoils are more important than those generated by ions. Moreover, one can notice that the profiles of phonons and vacancies do not exhibit Gaussian forms. Besides, the simulation shows that the defects which are due to ions are localized deeper in the target with regards to those enhanced by recoils. Indeed, from figures 4 & 5, we noticed that the phonons and vacancies which were due to recoils exhibited peaks at approximately 2000 Å under the surface sample. However, in the case of the generation by ions, the peaks (of phonons & vacancies) were observed at  $\sim 2200$  Å which was slightly inferior to the projected range  $R_p$ .

Besides, if we consider the redistribution of figure 4, one can suppose that the target temperature is largely elevated (until the fusion temperature of the substrate). This is not true because no such effect has been reported in literature [14].

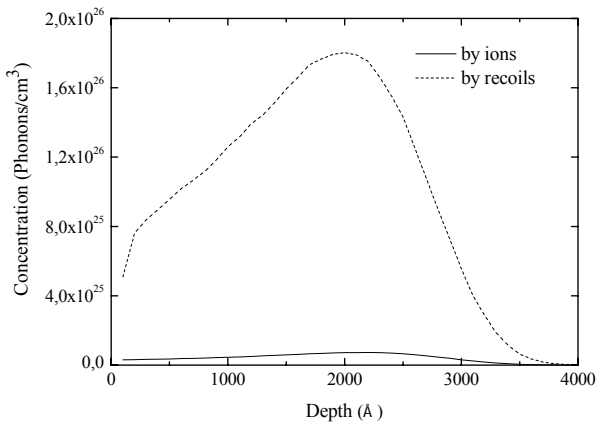


Figure 4: SRIM predictions of phonons profiles generated in silicon target implanted with carbon ions. The dose and

energy were fixed to  $2.7 \times 10^{17} \text{ C}^+ \text{ cm}^{-2}$  and 80 keV respectively.

- (—) Distribution of phonons generated by ions;
- (---) distribution of phonons generated by recoiled atoms.

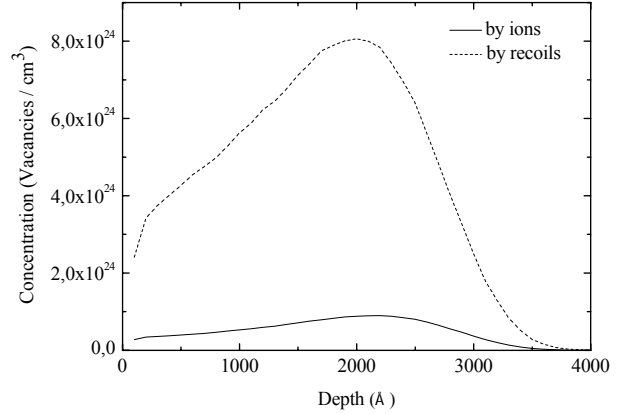


Figure 5: SRIM predictions of vacancies profiles generated in silicon target implanted with carbon ions. The dose and energy were fixed to  $2.7 \times 10^{17} \text{ C}^+ \text{ cm}^{-2}$  and 80 keV respectively.

- (—) Distribution of vacancies generated by ions;
- (---) distribution of vacancies generated by recoiled atoms.

## CONCLUSION

In this work several parameters related to carbon ion implantation, in silicon targets, were studied. The investigation was carried out by simulation, using the program SRIM2006. The redistribution of carbon ions in the target was obtained. It exhibited Gaussian-like distribution. The projected range and the standard deviation were slightly inferior to the experimental values provided in literature [14]. The difference was attributed to the fact that the simulated profile had not a perfect Gaussian shape. Indeed, we found that the peak was skewed towards the surface.

Concerning the defects profiles, the distribution shapes of phonons and vacancies in the target did not exhibit Gaussian forms. We note that the defects generated by

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recoils were predominant with regards to those generated by ions.

Finally, we note that SRIM code considers only amorphous targets. This means that if one is interested to study the ion implantation in crystalline targets, this should not be possible. Moreover, the SRIM simulates only as-implanted targets. In other words, the temperature effect is not taken into account by the code. Hence in such cases, one should use other codes or propose his own model.

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